



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:06 PM UTC

PDB ID : 7RF3 / pdb_00007rf3
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.26 Angstrom resolution
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Deposited on : 2021-07-13
Resolution : 2.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)

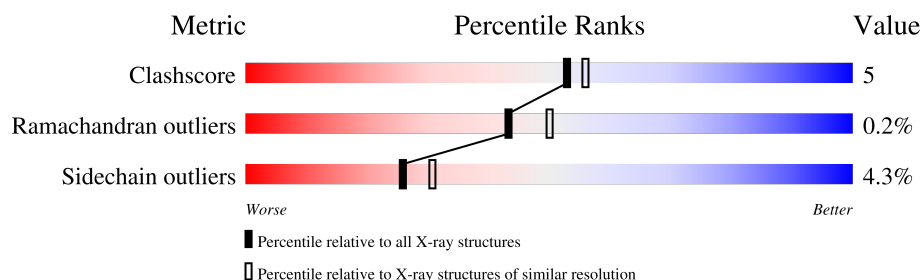
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

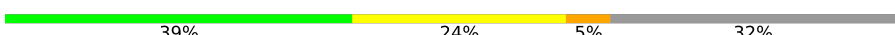
Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	344	86% 10% ..
1	a	344	85% 11% ..
2	B	510	87% 11% ..
2	b	510	87% 11% ..
3	C	461	87% 8% .
3	c	461	87% 10% ..

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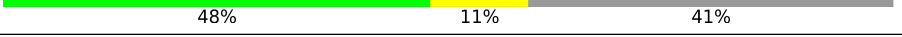
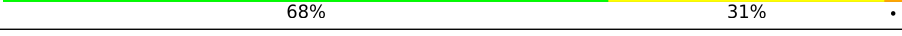
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	
14	r	41	
15	T	32	
15	t	32	
16	U	134	

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Mol	Chain	Length	Quality of chain
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	411	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	402	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103278 atoms, of which 51563 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7814	2610	3836	665	690	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6781	2249	3355	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3700	1168	1830	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3720	1170	1846	317	383			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
15	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

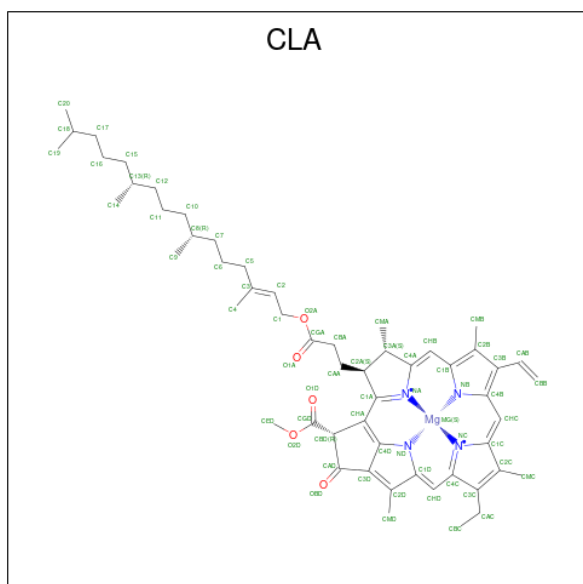
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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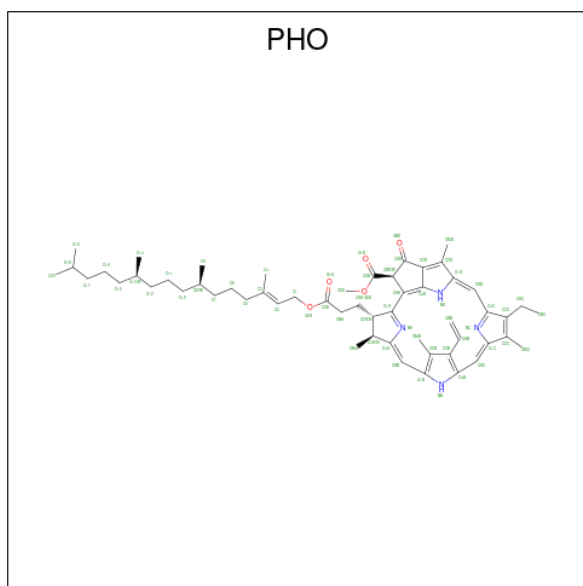
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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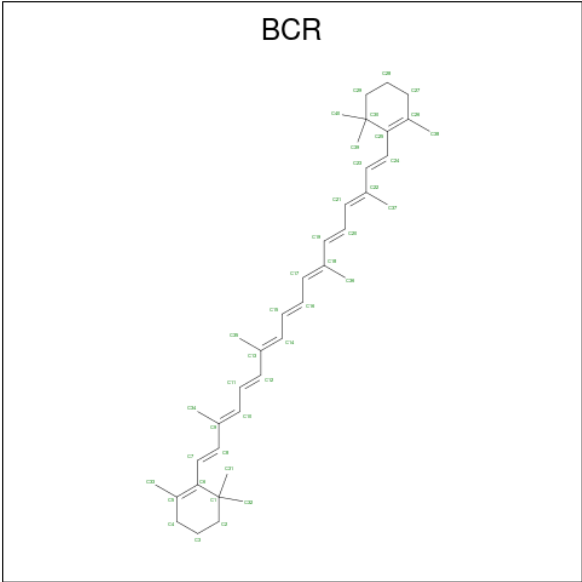
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	D	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
23	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	B	1	Total	C	H	0	0
			96	40	56		
24	C	1	Total	C	H	0	0
			96	40	56		
24	D	1	Total	C	H	0	0
			96	40	56		
24	H	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	K	1	Total	C	H	0	0
			96	40	56		
24	T	1	Total	C	H	0	0
			96	40	56		
24	Z	1	Total	C	H	0	0
			96	40	56		
24	a	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		
24	b	1	Total	C	H	0	0
			96	40	56		

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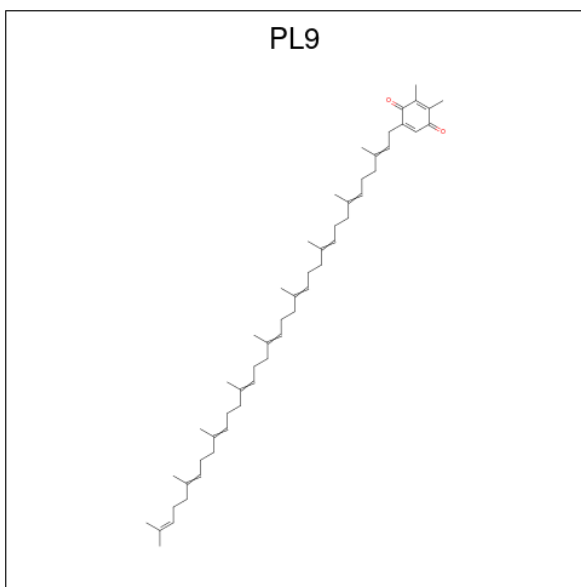
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		
24	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

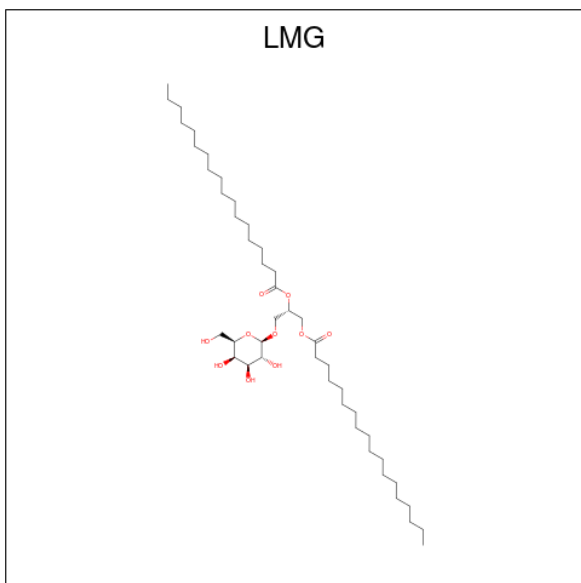
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



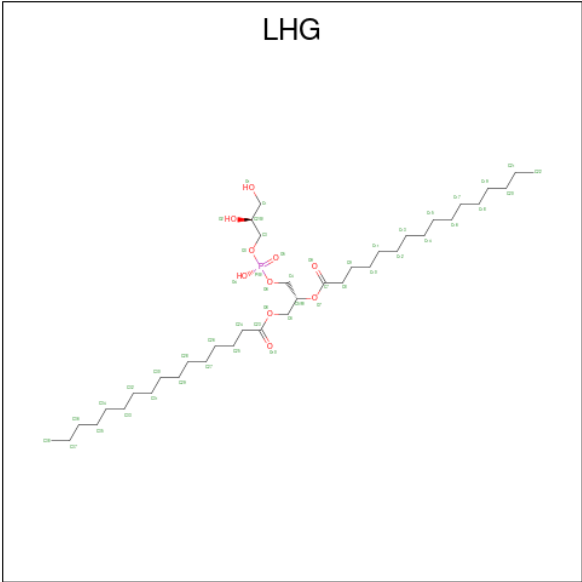
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



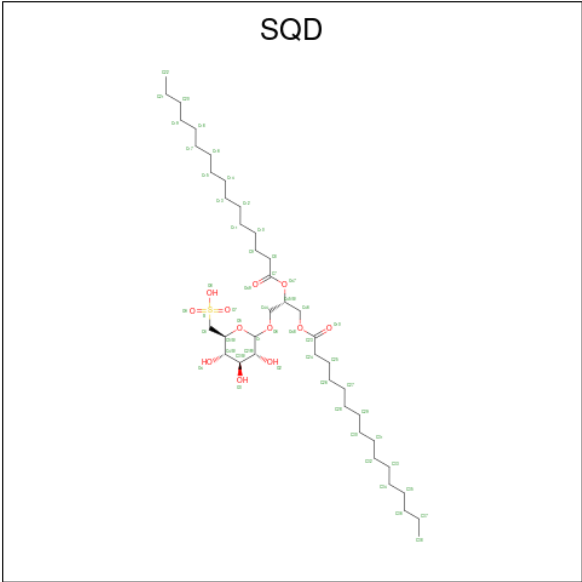
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			57	21	34	2		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



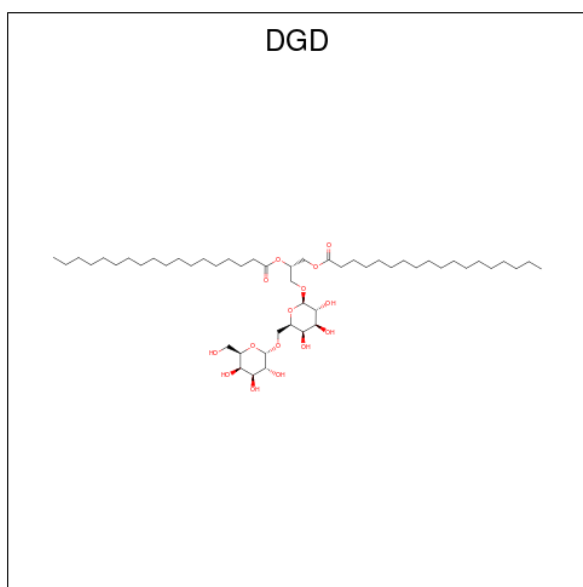
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	b	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
28	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



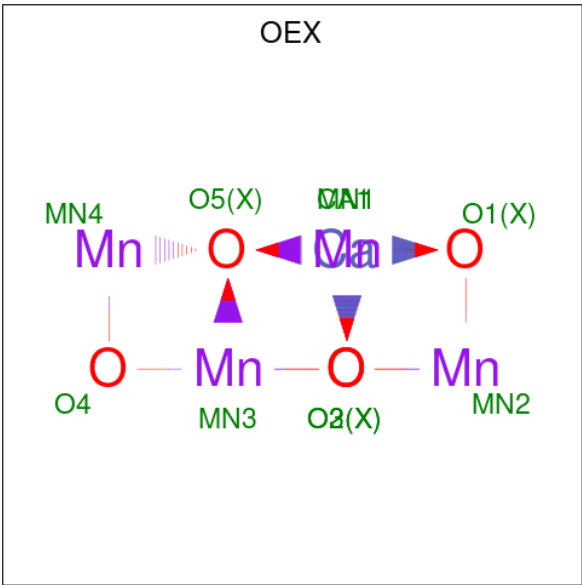
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



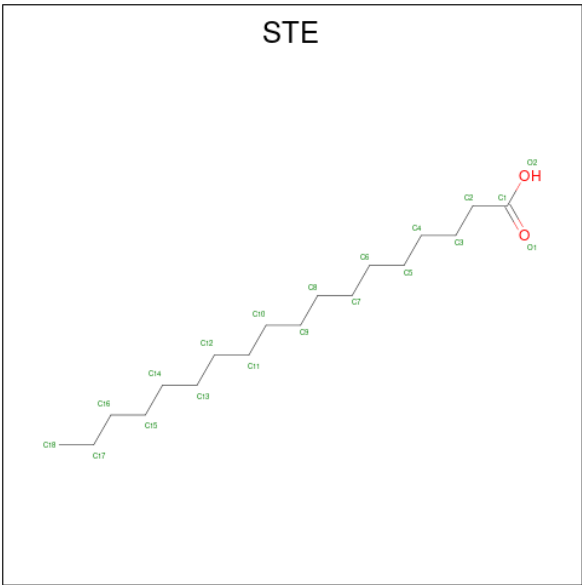
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	B	1	Total	C	H	O	0	0
			119	39	75	5		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		

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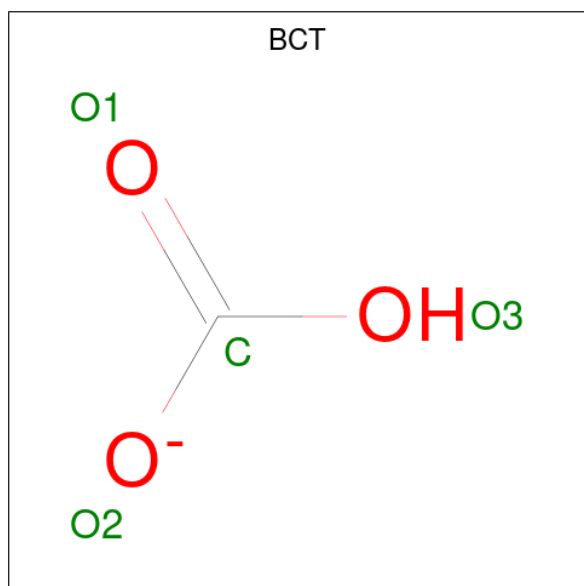
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 46 16 28 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 44 15 29	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0

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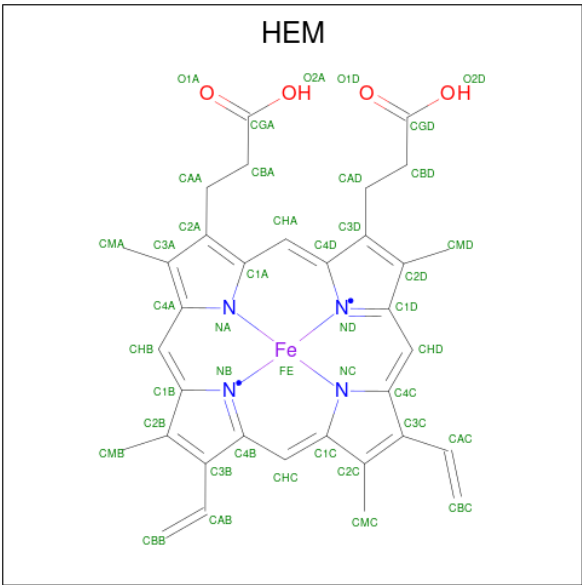
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	k	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		
32	t	1	Total	C	H		0	0
			26	10	16			
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



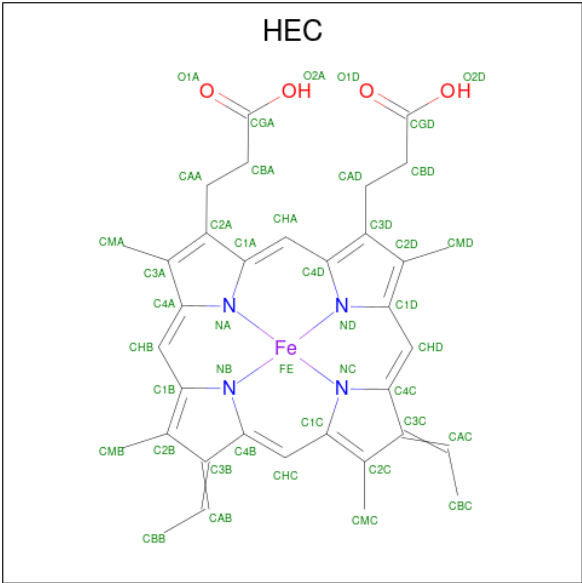
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
34	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	124	Total O 124 124	0	0
36	B	170	Total O 170 170	0	0
36	C	137	Total O 137 137	0	0
36	D	106	Total O 106 106	0	0
36	E	26	Total O 26 26	0	0
36	F	8	Total O 8 8	0	0
36	H	20	Total O 20 20	0	0
36	I	9	Total O 9 9	0	0
36	J	9	Total O 9 9	0	0
36	K	7	Total O 7 7	0	0
36	L	11	Total O 11 11	0	0
36	M	10	Total O 10 10	0	0
36	O	82	Total O 82 82	0	0
36	R	1	Total O 1 1	0	0
36	T	9	Total O 9 9	0	0
36	U	32	Total O 32 32	0	0
36	V	46	Total O 46 46	0	0
36	X	11	Total O 11 11	0	0
36	Y	3	Total O 3 3	0	0
36	Z	4	Total O 4 4	0	0
36	a	111	Total O 111 111	0	0

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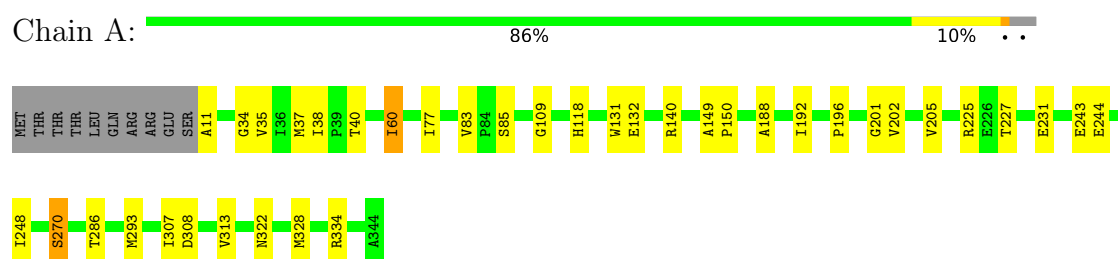
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	b	140	Total 140	O 140	0	0
36	c	115	Total 115	O 115	0	0
36	d	102	Total 102	O 102	0	0
36	e	19	Total 19	O 19	0	0
36	f	10	Total 10	O 10	0	0
36	h	22	Total 22	O 22	0	0
36	i	10	Total 10	O 10	0	0
36	j	10	Total 10	O 10	0	0
36	k	7	Total 7	O 7	0	0
36	l	7	Total 7	O 7	0	0
36	m	7	Total 7	O 7	0	0
36	o	79	Total 79	O 79	0	0
36	r	12	Total 12	O 12	0	0
36	t	10	Total 10	O 10	0	0
36	u	40	Total 40	O 40	0	0
36	v	39	Total 39	O 39	0	0
36	x	5	Total 5	O 5	0	0
36	y	5	Total 5	O 5	0	0
36	z	6	Total 6	O 6	0	0

3 Residue-property plots

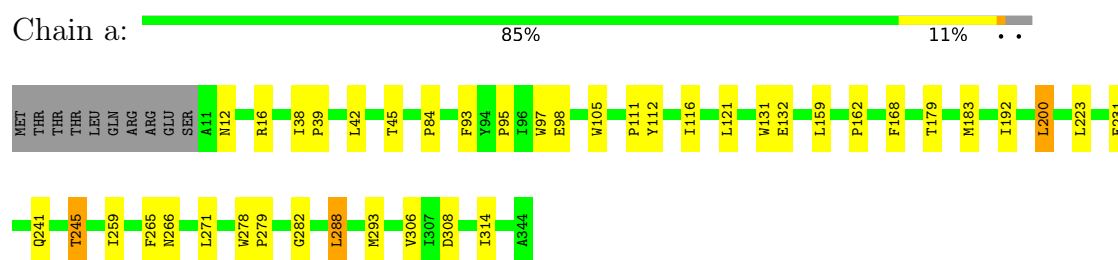
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

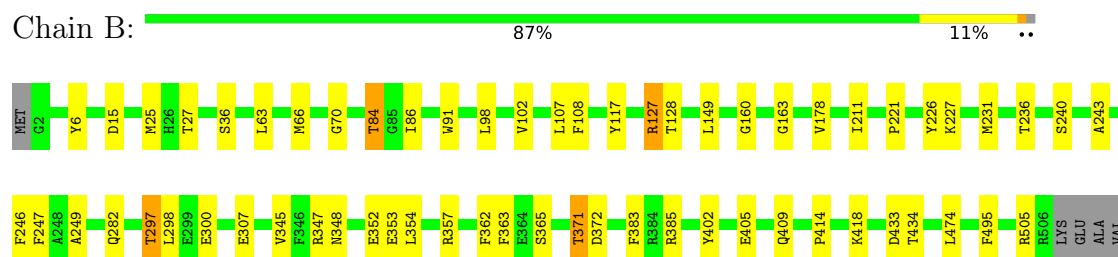
• Molecule 1: Photosystem II protein D1 1



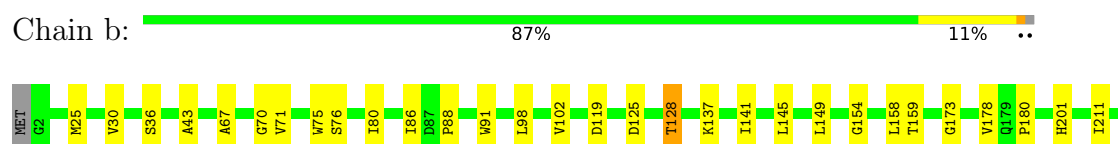
• Molecule 1: Photosystem II protein D1 1



• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein





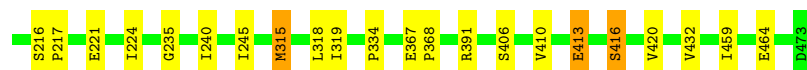
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 10% ..



• Molecule 4: Photosystem II D2 protein

Chain D: 88% 9% .



• Molecule 4: Photosystem II D2 protein

Chain d: 83% 12% ..



• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 86% 11% ..



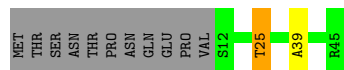
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  71% 25% ..



- Molecule 6: Cytochrome b559 subunit beta

Chain F:  71% .. 24%



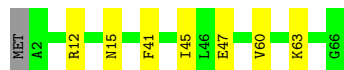
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  62% 9% . 24%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  88% 11% .



- Molecule 7: Photosystem II reaction center protein H

Chain h:  80% 14% . 5%



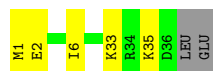
- Molecule 8: Photosystem II reaction center protein I

Chain I:  89% 5% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  82% 13% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  72% 18% 10%



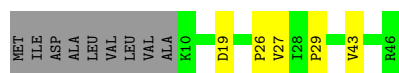
- Molecule 9: Photosystem II reaction center protein J

Chain j:  65% 22% 10%

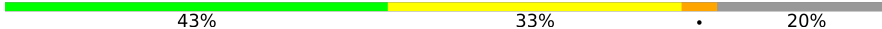


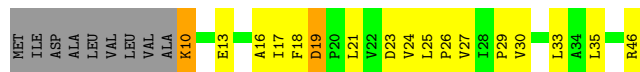
- Molecule 10: Photosystem II reaction center protein K

Chain K:  70% 11% 20%



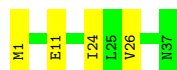
- Molecule 10: Photosystem II reaction center protein K

Chain k:  43% 33% 20%



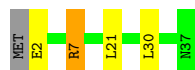
- Molecule 11: Photosystem II reaction center protein L

Chain L:  89% 11%



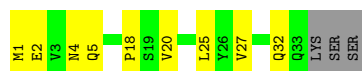
- Molecule 11: Photosystem II reaction center protein L

Chain l:  86% 8% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain M:  67% 25% 8%



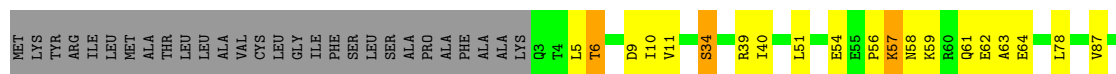
- Molecule 12: Photosystem II reaction center protein M

Chain m:  72% 14% 11%



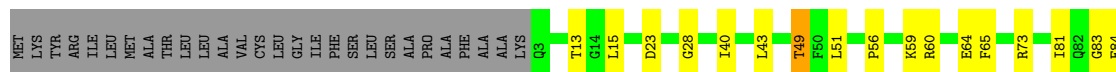
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  76% 12% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  76% 12% 10%

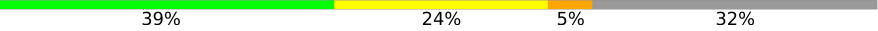


- Molecule 14: Photosystem II protein Y

Chain R:  49% 20% 32%



- Molecule 14: Photosystem II protein Y

Chain r:  39% 24% 5% 32%



- Molecule 15: Photosystem II reaction center protein T

Chain T:  81% 9% 6%



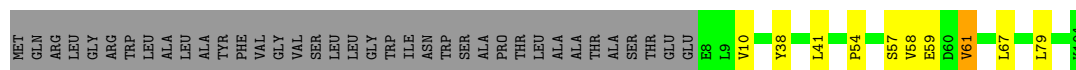
- Molecule 15: Photosystem II reaction center protein T

Chain t:  84% 9% 6%



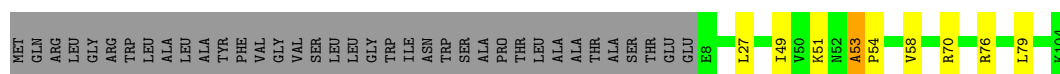
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U: 65% 7% 28%



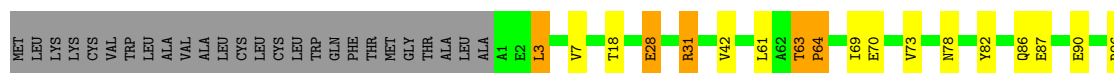
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u: 66% 6% 28%



- Molecule 17: Cytochrome c-550

Chain V: 70% 11% 16%



- Molecule 17: Cytochrome c-550

Chain v: 70% 12% 16%



- Molecule 18: Photosystem II reaction center X protein

Chain X: 76% 17% 7%

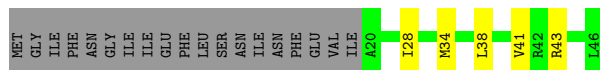


- Molecule 18: Photosystem II reaction center X protein

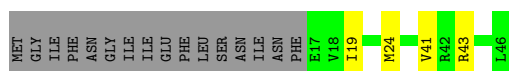
Chain x: 78% 17% 5%



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 221.64Å 307.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.26	Depositor
% Data completeness (in resolution range)	99.8 (33.54-2.26)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.238	Depositor
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.248	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	103278	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, PHO, STE, CL, OEX, LMG, HEM, BCR, BCT, FME, HEC, CLA, SQD, PL9, DGD, LHG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/2707 (0.0%)	0.67	0/3692
1	a	0.58	0/2704	0.65	0/3688
2	B	0.56	0/4161	0.63	0/5669
2	b	0.53	0/4118	0.62	0/5611
3	C	0.54	0/3547	0.62	0/4830
3	c	0.50	0/3619	0.60	0/4926
4	D	0.58	0/2812	0.64	0/3832
4	d	0.56	0/2821	0.65	0/3844
5	E	0.45	0/688	0.54	0/940
5	e	0.43	0/683	0.57	0/932
6	F	0.48	0/284	0.60	0/387
6	f	0.51	0/284	0.62	0/387
7	H	0.59	0/523	0.59	0/713
7	h	0.50	0/511	0.59	0/697
8	I	0.55	0/293	0.65	0/396
8	i	0.55	0/293	0.53	0/396
9	J	0.45	0/263	0.54	0/356
9	j	0.40	0/263	0.55	0/356
10	K	0.44	0/303	0.63	0/416
10	k	0.41	0/303	0.54	0/416
11	L	0.62	0/311	0.62	0/422
11	l	0.60	0/303	0.63	0/412
12	M	0.65	0/249	0.66	0/341
12	m	0.59	0/244	0.64	0/334
13	O	0.54	0/1904	0.65	0/2585
13	o	0.56	0/1905	0.64	0/2583
14	R	0.41	0/227	0.54	0/313
14	r	0.36	0/227	0.45	0/313
15	T	0.60	0/257	0.60	0/349
15	t	0.60	0/255	0.58	0/346
16	U	0.51	0/785	0.60	0/1064
16	u	0.54	0/785	0.64	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.54	0/1085	0.63	0/1473
17	v	0.52	0/1085	0.58	0/1473
18	X	0.45	0/284	0.58	0/384
18	x	0.39	0/289	0.49	0/391
19	Y	0.43	0/197	0.51	0/264
19	y	0.35	0/219	0.47	0/294
20	Z	0.40	0/490	0.50	0/669
20	z	0.35	0/488	0.44	0/666
All	All	0.54	1/42769 (0.0%)	0.62	0/58224

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
17	V	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	-7.55	1.50	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2519	2519	23	0
1	a	2619	2510	2510	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4005	3873	3867	42	0
2	b	3978	3836	3836	37	0
3	C	3426	3355	3343	25	0
3	c	3500	3426	3426	28	0
4	D	2717	2621	2621	22	0
4	d	2723	2627	2627	31	0
5	E	666	651	651	7	0
5	e	664	648	648	18	0
6	F	275	282	282	2	0
6	f	275	282	282	5	0
7	H	510	532	532	5	0
7	h	498	518	518	5	0
8	I	296	311	311	0	0
8	i	296	311	311	2	0
9	J	257	268	268	5	0
9	j	257	268	268	7	0
10	K	293	305	305	1	0
10	k	293	305	305	12	0
11	L	304	316	316	4	0
11	l	296	304	304	1	0
12	M	256	269	269	9	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	20	0
13	o	1874	1846	1846	21	0
14	R	221	238	238	3	0
14	r	221	238	238	7	0
15	T	258	261	261	5	0
15	t	256	256	256	1	0
16	U	774	773	773	5	0
16	u	774	773	773	5	1
17	V	1064	1071	1073	11	1
17	v	1064	1071	1073	14	0
18	X	281	312	312	4	0
18	x	286	316	314	4	0
19	Y	196	217	217	2	0
19	y	218	241	241	2	0
20	Z	479	516	516	8	0
20	z	477	509	509	11	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	2	0
22	B	1035	1139	1139	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	839	922	922	8	0
22	D	195	216	216	3	0
22	a	260	288	288	2	0
22	b	1035	1139	1139	15	0
22	c	839	919	919	15	0
22	d	130	144	144	4	0
23	A	64	74	74	0	0
23	D	64	74	74	1	0
23	a	64	74	74	1	0
23	d	64	74	74	1	0
24	A	40	56	56	0	0
24	B	120	168	168	4	0
24	C	40	56	56	1	0
24	D	40	56	56	1	0
24	H	40	56	56	0	0
24	K	80	112	112	2	0
24	T	40	56	56	3	0
24	Z	40	56	56	2	0
24	a	40	56	56	1	0
24	b	120	168	168	2	0
24	c	40	56	56	2	0
24	d	40	56	56	3	0
24	k	120	168	168	0	0
24	t	40	56	56	3	0
24	x	40	56	56	1	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	3	0
26	D	55	80	80	1	0
26	a	55	80	80	3	0
26	d	55	80	80	0	0
27	A	48	66	66	3	0
27	C	48	66	66	1	0
27	D	112	157	156	1	0
27	M	51	72	72	1	0
27	a	49	68	68	0	0
27	b	55	86	86	0	0
27	c	85	113	113	1	0
27	d	67	92	92	1	0
27	m	51	72	72	0	0
28	A	47	67	67	2	0
28	B	49	74	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	49	74	74	2	0
28	E	49	74	74	2	0
28	L	49	74	74	6	0
28	b	49	74	74	1	0
28	d	88	125	125	5	0
28	e	42	57	57	3	0
28	l	49	74	74	1	0
29	A	91	135	135	5	0
29	B	54	78	77	1	0
29	F	36	45	45	0	0
29	L	49	65	64	2	0
29	a	90	133	132	6	0
29	f	41	48	48	2	0
30	A	66	96	96	3	0
30	B	44	75	75	4	0
30	C	186	245	243	6	0
30	H	62	82	81	1	0
30	c	186	246	244	4	0
30	h	62	82	81	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	B	75	117	114	5	0
32	C	40	63	60	0	0
32	D	20	35	35	3	0
32	E	12	16	16	0	0
32	H	18	35	35	3	0
32	I	15	26	26	1	0
32	J	12	16	16	1	0
32	M	40	67	64	1	0
32	a	12	16	16	0	0
32	b	82	141	138	5	0
32	c	20	35	35	0	0
32	d	17	26	26	0	0
32	j	12	16	16	1	0
32	k	12	16	16	2	0
32	l	18	35	35	1	0
32	m	12	16	16	0	0
32	t	24	36	36	0	0
32	x	20	35	35	2	0
33	D	4	1	1	1	0
33	a	4	1	1	0	0
34	F	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	e	43	30	30	4	0
35	V	43	30	30	1	0
35	v	43	30	30	0	0
36	A	124	0	0	7	0
36	B	170	0	0	13	0
36	C	137	0	0	4	0
36	D	106	0	0	6	0
36	E	26	0	0	1	0
36	F	8	0	0	0	0
36	H	20	0	0	1	0
36	I	9	0	0	0	0
36	J	9	0	0	1	0
36	K	7	0	0	0	0
36	L	11	0	0	1	0
36	M	10	0	0	2	0
36	O	82	0	0	3	0
36	R	1	0	0	0	0
36	T	9	0	0	4	0
36	U	32	0	0	1	0
36	V	46	0	0	3	0
36	X	11	0	0	0	0
36	Y	3	0	0	0	0
36	Z	4	0	0	0	0
36	a	111	0	0	4	0
36	b	140	0	0	5	0
36	c	115	0	0	1	0
36	d	102	0	0	1	0
36	e	19	0	0	3	0
36	f	10	0	0	0	0
36	h	22	0	0	0	0
36	i	10	0	0	0	0
36	j	10	0	0	1	0
36	k	7	0	0	2	0
36	l	7	0	0	1	0
36	m	7	0	0	0	0
36	o	79	0	0	5	0
36	r	12	0	0	0	0
36	t	10	0	0	0	0
36	u	40	0	0	0	0
36	v	39	0	0	3	0
36	x	5	0	0	0	0
36	y	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	z	6	0	0	0	0
All	All	51715	51563	51525	508	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ASP:OD1	36:B:704:HOH:O	1.88	0.92
2:B:354:LEU:O	36:B:702:HOH:O	1.87	0.91
2:B:84:THR:O	36:B:703:HOH:O	1.87	0.91
11:L:11:GLU:OE1	36:L:201:HOH:O	1.88	0.90
1:a:266:ASN:ND2	36:a:501:HOH:O	2.01	0.89
17:v:75:TYR:OH	36:v:301:HOH:O	1.91	0.87
4:d:336:HIS:NE2	36:d:501:HOH:O	2.10	0.85
17:V:18:THR:OG1	36:V:301:HOH:O	1.94	0.84
1:A:244:GLU:O	36:A:501:HOH:O	1.96	0.84
17:V:128:ASP:OD1	36:V:302:HOH:O	1.94	0.84
15:T:2:GLU:OE2	36:T:201:HOH:O	1.96	0.84
32:B:624:STE:O2	36:B:705:HOH:O	1.94	0.84
9:j:36:LEU:O	36:j:201:HOH:O	1.96	0.83
29:B:622:SQD:O2	36:B:706:HOH:O	1.95	0.82
30:B:623:DGD:O3G	36:B:707:HOH:O	1.98	0.82
28:e:102:LHG:O5	36:e:201:HOH:O	1.97	0.82
13:o:28:GLY:O	36:o:302:HOH:O	1.99	0.79
10:k:46:ARG:O	36:k:201:HOH:O	2.01	0.78
13:O:124:ASN:ND2	36:O:301:HOH:O	2.10	0.77
10:k:23:ASP:OD2	36:k:202:HOH:O	2.02	0.75
7:H:47:GLU:OE2	36:H:201:HOH:O	2.07	0.73
16:u:53:ALA:HB1	16:u:54:PRO:HD2	1.72	0.72
2:B:347:ARG:NE	36:B:701:HOH:O	1.82	0.71
1:A:334:ARG:NH2	36:A:504:HOH:O	2.23	0.71
5:e:7:GLU:OE2	36:e:202:HOH:O	2.10	0.69
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.58	0.68
11:l:7:ARG:NH1	36:l:201:HOH:O	2.25	0.68
3:c:78:GLU:OE1	17:v:106:ASN:ND2	2.27	0.68
1:A:11:ALA:N	36:A:505:HOH:O	2.27	0.68
9:J:15:THR:HG22	9:J:19:MET:HE2	1.76	0.67
30:A:414:DGD:HB41	32:I:101:STE:H62	1.77	0.67
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:225:MET:O	36:o:303:HOH:O	2.14	0.65
15:T:2:GLU:CG	36:T:201:HOH:O	2.44	0.64
15:T:2:GLU:HG3	36:T:201:HOH:O	1.97	0.64
17:V:109:GLU:OE1	36:V:303:HOH:O	2.15	0.64
1:A:225:ARG:NH1	36:A:506:HOH:O	2.31	0.63
28:E:101:LHG:H312	28:E:101:LHG:H251	1.81	0.63
10:k:13:GLU:N	10:k:13:GLU:OE1	2.32	0.63
4:D:189:HIS:O	36:D:501:HOH:O	2.15	0.63
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.81	0.63
13:O:231:HIS:HE1	36:O:322:HOH:O	1.82	0.63
22:B:602:CLA:H43	7:H:45:ILE:HG22	1.81	0.62
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.31	0.62
2:b:91:TRP:HE1	32:b:621:STE:H111	1.65	0.62
2:b:137:LYS:NZ	36:b:704:HOH:O	2.30	0.61
2:B:227:LYS:NZ	36:B:716:HOH:O	2.33	0.61
4:D:23:LYS:HE2	4:D:135:LEU:HD21	1.82	0.61
2:B:211:ILE:HG23	32:B:627:STE:H51	1.81	0.61
24:T:101:BCR:H311	24:T:101:BCR:HC8	1.82	0.61
12:M:32:GLN:O	36:M:201:HOH:O	2.16	0.60
34:e:101:HEM:HHC	34:e:101:HEM:HBB2	1.83	0.60
14:r:18:TRP:O	14:r:22:ASN:ND2	2.35	0.60
20:z:9:LEU:HD13	20:z:54:VAL:HG11	1.84	0.60
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.84	0.59
4:D:307:GLU:OE2	36:D:502:HOH:O	2.17	0.59
2:b:102:VAL:HG11	22:b:606:CLA:H142	1.83	0.59
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.85	0.59
9:J:36:LEU:O	36:J:201:HOH:O	2.17	0.59
1:a:16:ARG:NH2	36:a:504:HOH:O	2.35	0.59
2:B:357:ARG:NE	36:B:708:HOH:O	2.07	0.59
1:a:200:LEU:HD13	30:c:517:DGD:HAW2	1.85	0.58
5:e:57:ALA:H	5:e:60:GLN:HE21	1.51	0.58
17:V:87:GLU:OE1	17:V:96:ARG:NH1	2.36	0.58
2:b:119:ASP:OD1	36:b:701:HOH:O	2.17	0.58
13:O:189:ARG:HD2	36:O:302:HOH:O	2.04	0.58
29:a:413:SQD:O6	36:a:502:HOH:O	2.17	0.58
2:b:287:ARG:HD3	36:b:711:HOH:O	2.04	0.58
16:U:54:PRO:O	36:U:201:HOH:O	2.17	0.57
17:v:77:LYS:HG2	17:v:95:LEU:HD12	1.86	0.57
26:a:410:PL9:H28	28:e:102:LHG:H201	1.87	0.57
24:B:619:BCR:H382	29:a:413:SQD:H82	1.86	0.57
32:B:624:STE:C1	36:B:705:HOH:O	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:414:DGD:HE4	2:b:76:SER:HB3	1.87	0.57
3:c:88:LEU:HB3	22:c:503:CLA:HED3	1.87	0.57
1:A:244:GLU:OE1	36:A:502:HOH:O	2.16	0.56
2:B:149[B]:LEU:HG	22:B:604:CLA:H18	1.87	0.56
30:A:414:DGD:HD5	2:b:75:TRP:HB3	1.87	0.56
2:b:307:GLU:OE2	36:b:702:HOH:O	2.18	0.56
20:z:19:MET:HE1	20:z:47:TRP:HB2	1.88	0.56
22:d:403:CLA:H92	18:x:18:ALA:HB2	1.88	0.56
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.88	0.56
8:i:33:LYS:O	8:i:35:LYS:NZ	2.39	0.56
12:M:5:GLN:HB2	36:M:202:HOH:O	2.06	0.56
2:B:91:TRP:HE1	32:B:620:STE:H32	1.72	0.55
2:b:159:THR:O	2:b:180:PRO:HB3	2.05	0.55
4:d:259:ILE:HD12	28:d:406:LHG:H291	1.88	0.55
24:t:101:BCR:H23C	24:t:101:BCR:H382	1.89	0.55
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.89	0.55
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.88	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.88	0.55
32:D:412:STE:H112	18:X:16:SER:HB3	1.89	0.55
5:e:63:ILE:HG22	5:e:64:PRO:HD2	1.89	0.55
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.89	0.54
2:B:371:THR:HG23	2:B:372:ASP:O	2.07	0.54
34:F:101:HEM:HBB2	34:F:101:HEM:HMB2	1.89	0.54
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.89	0.54
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.90	0.54
23:a:404:PHO:HBC2	23:a:404:PHO:HHD	1.89	0.54
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.07	0.53
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.43	0.53
9:j:18:GLY:O	9:j:22:ILE:HD13	2.08	0.53
3:C:148:GLY:O	3:C:156:LYS:NZ	2.41	0.53
1:a:179:THR:O	1:a:183:MET:HG3	2.08	0.53
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.91	0.53
20:z:32:ASP:HA	20:z:35:ARG:HG3	1.90	0.53
22:B:601:CLA:H51	32:H:103:STE:H151	1.91	0.53
17:v:104:MET:HA	17:v:107:LEU:HD22	1.90	0.53
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.08	0.53
13:o:189:ARG:NE	36:o:305:HOH:O	2.35	0.53
2:b:293:ALA:O	36:b:703:HOH:O	2.19	0.53
2:B:127:ARG:HG3	2:B:128:THR:HG23	1.91	0.52
3:C:126:GLY:O	3:C:130:VAL:HG13	2.09	0.52
2:b:211:ILE:HG23	32:b:626:STE:H31	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.92	0.52
22:B:611:CLA:H142	28:L:102:LHG:H371	1.91	0.52
13:O:51:LEU:HB2	13:O:234:LYS:HB3	1.91	0.52
2:b:36:SER:OG	24:b:618:BCR:H362	2.10	0.52
13:o:87:VAL:N	36:o:301:HOH:O	1.92	0.52
1:A:227:THR:HB	1:A:231:GLU:HG3	1.92	0.52
2:B:357:ARG:NH2	36:B:708:HOH:O	2.41	0.52
9:J:19:MET:O	9:J:23:VAL:HG23	2.10	0.52
4:d:194:ASN:HA	4:d:295:SER:OG	2.10	0.52
2:b:355:PHE:HE1	2:b:373:LYS:HG2	1.75	0.52
3:c:318:LEU:C	3:c:318:LEU:HD23	2.36	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.45	0.51
26:D:407:PL9:H322	28:L:102:LHG:H223	1.92	0.51
14:R:8:VAL:O	14:R:11:PRO:HD2	2.10	0.51
20:Z:51:VAL:O	20:Z:54:VAL:O	2.27	0.51
2:b:442:ILE:HD12	4:d:299:ILE:HG12	1.91	0.51
22:B:611:CLA:H71	28:L:102:LHG:H321	1.91	0.51
23:d:401:PHO:H3A	22:d:402:CLA:H142	1.91	0.51
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.92	0.51
15:T:25:GLU:OE1	36:T:202:HOH:O	2.19	0.51
4:d:246:MET:HE3	4:d:264:LYS:HD2	1.92	0.51
29:L:101:SQD:H102	22:b:614:CLA:H43	1.91	0.51
12:M:5:GLN:HE22	32:M:104:STE:C1	2.23	0.51
4:d:85:MET:HE3	4:d:107:LEU:HB3	1.92	0.51
20:z:32:ASP:N	20:z:32:ASP:OD1	2.43	0.51
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.46	0.51
3:c:406:SER:HA	3:c:420:VAL:HG23	1.92	0.51
5:e:68:ASP:O	5:e:72:ALA:HB2	2.11	0.50
10:k:21:LEU:HB2	19:y:24:MET:HE3	1.93	0.50
20:z:10:ALA:O	20:z:14:ILE:HG12	2.11	0.50
1:a:282:GLY:HA2	29:a:412:SQD:H223	1.92	0.50
2:b:67:ALA:HA	2:b:71:VAL:O	2.12	0.50
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.94	0.50
2:b:359:MET:HB2	2:b:425:ILE:HD12	1.92	0.50
4:d:49:LEU:HD13	24:d:404:BCR:C15	2.42	0.50
17:v:95:LEU:HD11	17:v:112:LEU:HD11	1.93	0.50
28:B:621:LHG:H161	28:L:102:LHG:H292	1.93	0.50
3:c:213:LEU:HD21	24:c:514:BCR:C20	2.41	0.50
17:V:28:GLU:HG3	17:V:31:ARG:HH12	1.75	0.50
3:c:315:MET:HE3	3:c:319:ILE:HD11	1.94	0.50
3:C:394:GLU:OE1	36:C:601:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:571:HOH:O	13:O:107:THR:HG21	2.11	0.49
34:e:101:HEM:HMC1	34:e:101:HEM:HBC2	1.94	0.49
3:c:48:LYS:NZ	36:c:606:HOH:O	2.41	0.49
3:c:334:PRO:HA	13:o:153:THR:OG1	2.13	0.49
3:C:48:LYS:NZ	36:C:610:HOH:O	2.45	0.49
22:C:511:CLA:H143	20:Z:20:VAL:HG13	1.93	0.49
20:z:1:MET:O	20:z:4:LEU:N	2.46	0.49
30:C:516:DGD:HA61	30:C:516:DGD:HAW1	1.95	0.49
2:b:141:ILE:HD11	7:h:14:LEU:HD22	1.95	0.49
22:b:615:CLA:HHC	22:b:615:CLA:HBB1	1.94	0.49
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.48	0.49
29:f:101:SQD:H372	18:x:27:VAL:HG21	1.94	0.49
22:b:605:CLA:HMA1	22:b:606:CLA:H3A	1.95	0.49
13:O:56:PRO:O	13:O:58:ASN:N	2.46	0.48
1:a:16:ARG:HB3	1:a:16:ARG:NH1	2.28	0.48
17:v:2:GLU:HB2	36:v:322:HOH:O	2.12	0.48
1:A:270:SER:HB3	29:A:412:SQD:O49	2.13	0.48
24:t:101:BCR:C8	24:t:101:BCR:H311	2.43	0.48
27:A:410:LMG:H321	3:C:217:PRO:HD3	1.96	0.48
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.47	0.48
14:r:6:LEU:HD12	14:r:10:LEU:HD23	1.96	0.48
2:B:249:ALA:HB2	22:B:604:CLA:HBC3	1.95	0.48
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.48	0.48
29:L:101:SQD:H202	24:T:101:BCR:H351	1.96	0.48
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.95	0.48
4:D:267:LEU:C	4:D:267:LEU:HD23	2.39	0.48
6:f:26:LEU:O	6:f:29:PRO:HD2	2.14	0.48
17:v:41:HIS:HA	17:v:45:ILE:O	2.14	0.48
2:B:347:ARG:CD	36:B:701:HOH:O	2.46	0.48
35:V:201:HEC:HMC1	35:V:201:HEC:HBC3	1.96	0.48
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.44	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.49	0.48
4:d:126:MET:HE3	4:d:143:ALA:O	2.13	0.48
13:o:23:ASP:HB2	36:o:343:HOH:O	2.13	0.48
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.95	0.48
22:c:508:CLA:H191	30:c:516:DGD:HA72	1.96	0.48
6:f:24:HIS:O	6:f:28:VAL:HG13	2.14	0.48
22:c:501:CLA:C3D	22:c:503:CLA:H2	2.44	0.47
22:B:613:CLA:H171	24:B:618:BCR:H312	1.97	0.47
13:O:34:SER:HB3	13:O:87:VAL:HG11	1.96	0.47
5:e:63:ILE:CG2	5:e:64:PRO:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:43:LEU:O	7:h:47:GLU:HG3	2.14	0.47
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.96	0.47
3:c:26:ARG:HA	22:c:511:CLA:OBD	2.15	0.47
29:f:101:SQD:H322	29:f:101:SQD:H371	1.97	0.47
5:e:64:PRO:HB2	5:e:79:PHE:CD2	2.49	0.47
13:o:13:THR:OG1	13:o:15:LEU:HD12	2.15	0.47
17:v:10:VAL:HG23	17:v:69:ILE:HD11	1.96	0.47
3:C:32:GLY:N	36:C:612:HOH:O	2.47	0.47
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.15	0.47
2:B:63:LEU:HA	2:B:66:MET:HE3	1.97	0.47
2:b:231:MET:HG2	22:b:610:CLA:HBC3	1.97	0.47
1:a:265:PHE:CD1	1:a:271:LEU:HD23	2.50	0.47
28:l:101:LHG:H271	12:m:22:LEU:HD21	1.97	0.47
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.96	0.47
3:C:334:PRO:HA	13:O:153:THR:OG1	2.14	0.47
4:D:307:GLU:HG3	36:D:502:HOH:O	2.15	0.47
10:k:10:LYS:HD2	10:k:10:LYS:N	2.30	0.47
12:m:9:ILE:HG13	12:m:13:LEU:HD22	1.96	0.47
1:A:85:SER:HA	1:A:109:GLY:HA3	1.97	0.46
2:B:495:PHE:HD1	2:B:505:ARG:NH1	2.13	0.46
5:E:68:ASP:O	5:E:72:ALA:HB2	2.15	0.46
2:b:275:TRP:CE2	2:b:315:ILE:HG13	2.49	0.46
3:c:45:LEU:HA	3:c:139:THR:HG22	1.97	0.46
22:B:601:CLA:O1D	22:B:601:CLA:H2A	2.15	0.46
12:M:4:ASN:HD21	27:M:101:LMG:C28	2.28	0.46
4:d:79:SER:HA	4:d:172:SER:HB3	1.97	0.46
5:e:26:THR:HA	14:r:15:ALA:HB1	1.98	0.46
17:V:69:ILE:O	17:V:73:VAL:HG23	2.16	0.46
3:c:213:LEU:HD21	24:c:514:BCR:H20C	1.97	0.46
2:B:117:TYR:HA	11:L:1:MET:HE1	1.98	0.46
16:U:58:VAL:O	16:U:61:VAL:HG22	2.15	0.46
2:b:201:HIS:HB2	22:b:602:CLA:CHB	2.45	0.46
4:d:241:GLU:CD	4:d:241:GLU:H	2.24	0.46
2:B:160:GLY:HA2	2:B:163:GLY:O	2.16	0.46
30:B:623:DGD:O1G	30:B:623:DGD:O1B	2.33	0.46
1:a:97:TRP:HA	8:i:1:FME:HG2	1.97	0.46
3:c:42:LEU:HD21	22:c:511:CLA:H2A	1.98	0.46
17:v:6:GLU:OE1	17:v:6:GLU:N	2.46	0.46
17:v:76:MET:HE1	17:v:115:ILE:HD12	1.98	0.46
1:A:308:ASP:HB2	5:E:52:PRO:O	2.16	0.46
3:c:334:PRO:HA	13:o:153:THR:HG1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:99:GLY:HA3	32:x:102:STE:H151	1.98	0.46
10:k:16:ALA:O	10:k:19:ASP:HB2	2.15	0.46
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.46	0.46
32:B:627:STE:H71	32:H:103:STE:H32	1.98	0.46
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.31	0.46
34:e:101:HEM:HBD2	6:f:23:VAL:HG21	1.98	0.46
13:O:133:VAL:HG12	13:O:135:SER:H	1.81	0.45
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.51	0.45
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.45
5:e:77:GLU:CD	36:e:203:HOH:O	2.59	0.45
22:B:605:CLA:H61	22:B:605:CLA:H41	1.68	0.45
4:D:268:HIS:CE1	33:D:402:BCT:O1	2.69	0.45
29:a:412:SQD:H311	32:k:104:STE:H82	1.98	0.45
4:d:197:HIS:O	4:d:201:VAL:HG23	2.16	0.45
4:d:267:LEU:C	4:d:267:LEU:HD23	2.40	0.45
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.98	0.45
30:B:623:DGD:HB52	30:B:623:DGD:HB21	1.70	0.45
5:E:26:THR:HA	14:R:15:ALA:HB1	1.98	0.45
17:V:63:THR:HG22	17:V:64:PRO:CD	2.47	0.45
3:c:150:ASP:OD2	3:c:152:LYS:HB2	2.16	0.45
34:e:101:HEM:HBC2	34:e:101:HEM:CMC	2.46	0.45
13:o:40:ILE:HG21	13:o:43:LEU:HB2	1.99	0.45
1:A:201:GLY:HA3	1:A:286:THR:HB	1.98	0.45
2:B:297:THR:HG23	2:B:300:GLU:OE1	2.17	0.45
2:B:434:THR:OG1	13:O:178:LYS:NZ	2.50	0.45
10:k:17:ILE:HG13	10:k:18:PHE:CD1	2.52	0.45
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.98	0.45
13:O:56:PRO:HG3	13:O:63:ALA:H	1.82	0.45
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.99	0.45
3:C:318:LEU:C	3:C:318:LEU:HD23	2.41	0.45
22:C:510:CLA:H193	22:C:510:CLA:HBC3	1.98	0.45
13:O:5:LEU:HD13	13:O:10:ILE:HD11	1.98	0.45
22:b:615:CLA:H2	22:b:616:CLA:HBB2	1.99	0.45
28:d:407:LHG:H242	28:d:407:LHG:H272	1.78	0.45
17:V:3:LEU:HD23	17:V:3:LEU:HA	1.88	0.45
2:B:433:ASP:OD1	2:B:433:ASP:C	2.59	0.45
13:O:57:LYS:HE3	13:O:58:ASN:HB3	1.99	0.45
5:e:57:ALA:H	5:e:60:GLN:HG2	1.82	0.45
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.52	0.45
2:B:363:PHE:HB3	2:B:365:SER:O	2.17	0.45
3:c:167:VAL:HG12	22:c:512:CLA:H42	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:367:GLU:N	3:c:368:PRO:CD	2.80	0.45
4:d:91:LEU:HD12	7:h:52:THR:HG21	1.99	0.45
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.52	0.45
1:A:40:THR:O	1:A:118:HIS:HB3	2.17	0.44
2:B:102:VAL:HG11	22:B:606:CLA:H111	1.99	0.44
3:C:109:PHE:O	3:C:113:VAL:HG23	2.17	0.44
27:A:410:LMG:H391	3:C:281:MET:HG3	1.99	0.44
22:C:509:CLA:H91	22:C:509:CLA:H112	1.79	0.44
18:X:27:VAL:O	18:X:31:ILE:HG13	2.17	0.44
2:b:30:VAL:HG12	22:b:605:CLA:HHD	1.99	0.44
30:c:516:DGD:HAT1	30:c:517:DGD:HB82	1.97	0.44
2:b:25:MET:HG2	24:b:617:BCR:H23C	1.99	0.44
22:c:510:CLA:H191	10:k:33:LEU:HD22	1.99	0.44
13:o:178:LYS:HA	13:o:178:LYS:HD3	1.78	0.44
18:x:12:ILE:HD13	32:x:102:STE:H141	1.99	0.44
20:z:15:LEU:HG	20:z:19:MET:HE2	1.98	0.44
26:A:409:PL9:H261	28:E:101:LHG:H202	2.00	0.44
5:E:78:THR:O	5:E:82:GLN:HG3	2.17	0.44
4:d:261:PHE:CZ	28:d:406:LHG:HC81	2.52	0.44
14:r:20:VAL:O	14:r:24:LEU:HB2	2.17	0.44
1:a:105:TRP:CZ3	1:a:111:PRO:HG3	2.52	0.44
2:b:43:ALA:HA	32:b:625:STE:H31	1.99	0.44
3:c:38:GLY:HA3	22:c:511:CLA:HMD2	1.98	0.44
1:A:196:PRO:HB3	30:C:517:DGD:HA92	2.00	0.44
22:C:504:CLA:H101	30:C:517:DGD:HBN1	1.99	0.44
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.52	0.44
9:J:17:ALA:O	9:J:21:VAL:HG23	2.17	0.44
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.53	0.44
4:d:58:TRP:CZ2	5:e:63:ILE:HG23	2.53	0.44
24:B:617:BCR:H382	24:B:617:BCR:H23C	1.98	0.44
28:B:621:LHG:H222	12:M:18:PRO:HG3	1.98	0.44
28:D:409:LHG:H172	28:L:102:LHG:H212	1.98	0.44
17:V:122:GLU:N	17:V:123:PRO:HD2	2.32	0.44
16:u:27:LEU:HD22	16:u:49:ILE:HG21	1.99	0.44
1:A:60:ILE:HB	1:A:83:VAL:CG1	2.48	0.44
2:B:221:PRO:HA	22:B:609:CLA:HED3	2.00	0.44
22:B:615:CLA:H201	22:B:615:CLA:C1B	2.48	0.44
5:E:7:GLU:OE2	36:E:1401:HOH:O	2.21	0.44
3:c:68:THR:OG1	22:c:503:CLA:HED1	2.18	0.44
2:B:36:SER:OG	24:B:618:BCR:H362	2.17	0.44
22:B:603:CLA:C3D	22:B:605:CLA:H2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:623:DGD:HG2	30:B:623:DGD:HA22	2.00	0.44
3:C:419:PHE:HA	30:C:516:DGD:O3E	2.18	0.44
27:D:408:LMG:H112	36:D:515:HOH:O	2.18	0.44
12:M:27:VAL:HG13	32:l:102:STE:H71	2.00	0.44
22:b:610:CLA:H122	22:b:615:CLA:HAA1	2.00	0.44
4:d:179:PHE:O	4:d:182:LEU:HB2	2.17	0.44
3:c:459:ILE:HG21	3:c:464:GLU:HG3	2.00	0.43
4:d:272:LEU:C	4:d:272:LEU:HD23	2.43	0.43
1:A:202:VAL:HG11	22:A:403:CLA:C3D	2.48	0.43
2:B:307:GLU:OE1	13:o:59:LYS:HG2	2.18	0.43
2:b:317:ASN:HA	2:b:330:MET:HE1	1.99	0.43
5:e:23:HIS:HA	5:e:26:THR:OG1	2.19	0.43
20:z:36:SER:HA	20:z:39:LEU:HD23	1.99	0.43
2:B:433:ASP:O	36:B:709:HOH:O	2.20	0.43
13:O:6:THR:HG22	13:O:9:ASP:CG	2.43	0.43
4:d:42:TYR:CZ	6:f:25:THR:HG23	2.53	0.43
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.00	0.43
30:H:102:DGD:HB21	30:H:102:DGD:HB51	1.82	0.43
20:Z:31:GLN:CD	20:Z:32:ASP:H	2.25	0.43
24:d:404:BCR:H331	24:d:404:BCR:C8	2.48	0.43
26:A:409:PL9:H471	26:A:409:PL9:H451	1.78	0.43
2:B:6:TYR:OH	28:B:621:LHG:HC2	2.18	0.43
1:a:308:ASP:OD1	1:a:308:ASP:C	2.62	0.43
32:b:624:STE:H22	27:d:408:LMG:O9	2.18	0.43
3:c:128:GLY:HA3	22:c:513:CLA:C3C	2.48	0.43
22:B:601:CLA:H72	32:H:103:STE:H183	2.00	0.43
1:a:45:THR:HG23	22:a:411:CLA:H201	2.00	0.43
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.00	0.43
2:b:145:LEU:HB3	22:b:604:CLA:H161	2.00	0.43
28:A:411:LHG:H162	29:A:412:SQD:H131	1.99	0.43
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.54	0.43
1:a:308:ASP:HA	36:a:542:HOH:O	2.18	0.43
26:a:410:PL9:H253	28:e:102:LHG:H211	2.00	0.43
2:b:86:ILE:HD12	2:b:88:PRO:HD3	2.00	0.43
22:A:402:CLA:HBB1	22:A:402:CLA:HMB3	2.01	0.43
22:B:611:CLA:H203	22:B:613:CLA:H8	2.01	0.43
2:b:125:ASP:OD2	2:b:128:THR:HG23	2.18	0.43
4:d:62:GLY:HA2	5:e:63:ILE:HG21	2.01	0.43
24:K:101:BCR:H10C	19:Y:28:ILE:HG23	2.00	0.43
17:V:61:LEU:HB2	17:V:82:TYR:OH	2.18	0.43
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:d:403:CLA:H91	22:d:403:CLA:H111	1.88	0.43
1:A:307:ILE:HG22	1:A:313:VAL:HA	2.01	0.43
3:C:406:SER:HA	3:C:420:VAL:HG23	2.01	0.43
10:k:18:PHE:HE2	20:z:13:VAL:HG21	1.83	0.43
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.54	0.42
5:E:18:ARG:O	5:E:22[A]:ILE:HG22	2.19	0.42
19:Y:34:MET:O	19:Y:38:LEU:HG	2.19	0.42
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.07	0.42
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.01	0.42
16:u:53:ALA:HB1	16:u:54:PRO:CD	2.46	0.42
22:B:605:CLA:H92	22:B:605:CLA:H62	1.85	0.42
22:B:606:CLA:H161	22:B:606:CLA:H122	1.81	0.42
3:C:42:LEU:HD21	22:C:511:CLA:H2A	2.01	0.42
4:D:266:TRP:CD1	28:D:409:LHG:HC31	2.54	0.42
1:A:77:ILE:HD13	1:A:77:ILE:HA	1.93	0.42
24:D:406:BCR:H331	24:D:406:BCR:C8	2.48	0.42
20:Z:31:GLN:NE2	20:Z:32:ASP:HB2	2.34	0.42
2:b:246:PHE:CD1	2:b:246:PHE:C	2.96	0.42
28:A:411:LHG:C16	29:A:412:SQD:H131	2.49	0.42
2:B:247:PHE:CE1	22:B:602:CLA:H102	2.54	0.42
24:K:101:BCR:H312	20:Z:16:SER:HB3	2.01	0.42
1:a:288:LEU:HG	3:c:432:VAL:HG22	2.02	0.42
3:C:367:GLU:N	3:C:368:PRO:CD	2.82	0.42
9:j:17:ALA:O	9:j:21:VAL:HG12	2.19	0.42
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.01	0.42
2:B:474:LEU:O	4:D:134:ARG:NH1	2.49	0.42
3:C:67:MET:HB3	3:C:88:LEU:HD12	2.01	0.42
3:C:135:ARG:O	3:C:135:ARG:HD3	2.19	0.42
30:C:516:DGD:HA32	32:J:101:STE:H71	2.02	0.42
20:Z:11:ALA:O	20:Z:15:LEU:HB2	2.20	0.42
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.55	0.42
1:a:278:TRP:HB3	1:a:279:PRO:HD3	2.02	0.42
24:a:406:BCR:H24C	24:a:406:BCR:H371	1.86	0.42
19:y:41:VAL:C	19:y:43:ARG:H	2.25	0.42
22:B:613:CLA:H191	28:B:621:LHG:H223	2.02	0.42
22:B:614:CLA:H143	22:B:614:CLA:H111	1.86	0.42
3:C:262:ARG:NH2	36:C:604:HOH:O	2.30	0.42
4:D:307:GLU:CD	36:D:502:HOH:O	2.62	0.42
16:U:58:VAL:HG12	16:U:79:LEU:HD22	2.02	0.42
20:Z:9:LEU:HD13	20:Z:54:VAL:HG11	2.01	0.42
22:c:510:CLA:C2D	22:c:510:CLA:H193	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:81:GLU:O	5:e:84:LYS:HE2	2.18	0.42
29:A:412:SQD:H381	9:J:22:ILE:HD11	2.02	0.42
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.55	0.42
7:H:12:ARG:NH2	7:H:15:ASN:O	2.49	0.42
28:d:406:LHG:H281	15:t:17:PHE:CD1	2.54	0.42
13:o:121:THR:OG1	13:o:123:LYS:HG3	2.19	0.42
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.01	0.42
32:D:412:STE:H112	18:X:16:SER:CB	2.49	0.42
29:a:412:SQD:H381	9:j:22:ILE:HD11	2.02	0.42
29:a:412:SQD:H291	32:k:104:STE:H71	2.02	0.42
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.73	0.42
4:D:13:GLY:O	4:D:17:ILE:HG12	2.20	0.42
13:o:160:LYS:HD2	13:o:160:LYS:HA	1.91	0.42
22:C:502:CLA:H141	22:C:502:CLA:H161	1.84	0.41
22:c:511:CLA:H143	20:z:20:VAL:HG13	2.01	0.41
17:v:67:ASP:OD1	17:v:67:ASP:N	2.52	0.41
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.55	0.41
4:D:246:MET:HE3	4:D:264:LYS:HG2	2.02	0.41
11:L:26:VAL:HG11	28:L:102:LHG:H202	2.02	0.41
22:B:603:CLA:C2D	22:B:605:CLA:H2	2.50	0.41
4:D:296:TYR:CE2	4:D:319:LEU:HD22	2.55	0.41
14:R:20:VAL:O	14:R:24:LEU:HB2	2.20	0.41
3:c:217:PRO:HG3	30:c:515:DGD:HA81	2.02	0.41
3:c:245:ILE:HD13	27:c:520:LMG:H382	2.02	0.41
4:D:166:SER:OG	4:D:168:PHE:HB3	2.20	0.41
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.55	0.41
10:K:26:PRO:O	10:K:29:PRO:HD2	2.20	0.41
1:a:93:PHE:HZ	22:a:405:CLA:HAA1	1.85	0.41
1:a:112:TYR:O	1:a:116:ILE:HG12	2.20	0.41
3:c:27:ASP:CG	3:c:30:SER:HG	2.26	0.41
22:c:511:CLA:H122	20:z:24:PRO:HG3	2.02	0.41
7:h:25:TRP:O	7:h:26:GLY:C	2.62	0.41
17:v:21:LEU:HD11	17:v:117:GLY:HA3	2.03	0.41
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.41
4:d:126:MET:HA	4:d:129:GLN:OE1	2.19	0.41
32:D:412:STE:H181	18:X:21:LEU:HD21	2.02	0.41
11:L:24:ILE:HG12	12:M:18:PRO:HB2	2.02	0.41
2:b:414:PRO:HB2	2:b:415:PRO:HD3	2.02	0.41
16:u:70:ARG:HD2	16:u:70:ARG:HA	1.82	0.41
1:A:322:ASN:OD1	36:A:503:HOH:O	2.22	0.41
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:457:LYS:HE2	4:D:227:GLU:O	2.20	0.41
22:D:404:CLA:H141	22:D:404:CLA:H161	1.86	0.41
26:a:410:PL9:H201	26:a:410:PL9:H221	1.94	0.41
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.01	0.41
5:e:26:THR:HG22	14:r:15:ALA:HB1	2.03	0.41
9:j:26:GLY:HA2	32:j:101:STE:H62	2.03	0.41
10:k:24:VAL:O	10:k:27:VAL:HG22	2.21	0.41
10:k:26:PRO:O	10:k:29:PRO:HD2	2.21	0.41
22:B:614:CLA:H18	22:B:614:CLA:H152	1.87	0.41
24:Z:101:BCR:H11C	24:Z:101:BCR:H341	1.90	0.41
22:b:601:CLA:C3C	24:x:101:BCR:H21C	2.51	0.41
10:k:25:LEU:N	10:k:26:PRO:CD	2.84	0.41
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.51	0.41
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.02	0.41
22:C:507:CLA:H142	22:C:507:CLA:H111	1.95	0.41
30:C:516:DGD:HB72	27:C:518:LMG:H401	2.03	0.41
16:U:57:SER:HB2	16:U:59:GLU:OE1	2.21	0.41
24:Z:101:BCR:H24C	24:Z:101:BCR:H371	1.89	0.41
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.03	0.41
3:c:109:PHE:O	3:c:113:VAL:HG23	2.21	0.41
3:c:203:THR:O	3:c:235:GLY:HA3	2.21	0.41
22:c:501:CLA:H192	22:c:507:CLA:HBB1	2.01	0.41
22:c:502:CLA:H192	22:c:502:CLA:H162	1.91	0.41
4:d:103:ARG:O	4:d:107:LEU:HG	2.21	0.41
4:d:190:ASN:HB2	4:d:296:TYR:CD2	2.55	0.41
5:e:36:LEU:HA	5:e:39:SER:OG	2.21	0.41
13:o:60:ARG:HD2	13:o:60:ARG:HA	1.96	0.41
13:o:93:LEU:O	13:o:128:SER:HA	2.20	0.41
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.56	0.41
15:T:18:PHE:HB2	24:T:101:BCR:HC8	2.02	0.40
20:Z:15:LEU:HD22	20:Z:19:MET:HG3	2.04	0.40
22:b:601:CLA:H91	22:b:601:CLA:H111	1.91	0.40
17:v:90:GLU:HB2	36:v:331:HOH:O	2.21	0.40
26:A:409:PL9:H361	6:F:25:THR:HG21	2.03	0.40
29:A:413:SQD:H341	22:b:616:CLA:H93	2.03	0.40
1:a:306:VAL:HG12	1:a:314:ILE:HB	2.03	0.40
22:d:403:CLA:H152	7:h:36:GLY:HA3	2.03	0.40
5:e:40:THR:HB	14:r:4:ARG:HD2	2.03	0.40
3:C:168:LEU:HD21	22:C:509:CLA:H61	2.02	0.40
24:C:514:BCR:H24C	24:C:514:BCR:H371	1.92	0.40
4:D:272:LEU:HD23	4:D:272:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:LEU:HD22	23:D:401:PHO:HBC3	2.04	0.40
22:D:404:CLA:H193	22:D:404:CLA:H162	1.80	0.40
22:D:404:CLA:HBA1	22:D:404:CLA:C4A	2.51	0.40
13:O:130:GLN:OE1	13:O:130:GLN:HA	2.21	0.40
2:b:280:PHE:CD2	2:b:312:TYR:HB3	2.56	0.40
24:t:101:BCR:C23	24:t:101:BCR:C38	2.99	0.40
27:A:410:LMG:HC8	3:C:216:SER:HB2	2.04	0.40
2:B:345:VAL:HG13	2:B:353:GLU:OE2	2.21	0.40
2:B:347:ARG:HA	2:B:352:GLU:O	2.21	0.40
2:b:43:ALA:HB3	32:b:620:STE:H72	2.03	0.40
22:b:614:CLA:H203	22:b:614:CLA:H161	1.89	0.40
4:d:61:HIS:CE1	4:d:168:PHE:CE2	3.08	0.40
28:d:407:LHG:HC81	28:d:407:LHG:HC31	2.03	0.40
14:r:4:ARG:HA	14:r:7:VAL:HG22	2.03	0.40
1:A:140:ARG:HD3	36:D:589:HOH:O	2.21	0.40
2:B:414:PRO:O	2:B:418:LYS:HG3	2.21	0.40
22:B:606:CLA:H91	22:B:606:CLA:H112	1.68	0.40
4:D:79:SER:HA	4:D:172:SER:HB3	2.03	0.40
7:H:60:VAL:HG12	7:H:60:VAL:O	2.20	0.40
22:b:607:CLA:H93	22:b:607:CLA:H111	1.99	0.40
28:b:623:LHG:O4	4:d:141:TYR:OH	2.18	0.40
4:d:319:LEU:O	4:d:323:GLU:HG3	2.21	0.40
24:d:404:BCR:H402	9:j:21:VAL:HG21	2.03	0.40
13:o:83:GLY:HA2	13:o:98:GLU:HG3	2.04	0.40
13:o:84:GLU:OE2	13:o:86:LYS:NZ	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:70:GLU:OE2	16:u:76:ARG:HE[3_457]	1.56	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	40
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	442/461 (96%)	431 (98%)	10 (2%)	1 (0%)	43	50
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	50
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
13	O	243/272 (89%)	232 (96%)	8 (3%)	3 (1%)	10	7
13	o	242/272 (89%)	229 (95%)	11 (4%)	2 (1%)	16	14
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	17
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	2	1
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	3
20	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	5231/5700 (92%)	5087 (97%)	132 (2%)	12 (0%)	43	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER
16	u	53	ALA
3	C	416	SER
19	Y	43	ARG
20	Z	31	GLN
13	O	57	LYS
1	a	259	ILE
13	o	73	ARG
13	o	56	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	264 (98%)	6 (2%)	45	56
1	a	269/280 (96%)	260 (97%)	9 (3%)	33	42
2	B	408/407 (100%)	395 (97%)	13 (3%)	34	43
2	b	402/407 (99%)	391 (97%)	11 (3%)	39	49
3	C	346/362 (96%)	339 (98%)	7 (2%)	48	59
3	c	354/362 (98%)	338 (96%)	16 (4%)	24	29
4	D	276/283 (98%)	272 (99%)	4 (1%)	59	70
4	d	277/283 (98%)	262 (95%)	15 (5%)	20	21
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	48
5	e	71/73 (97%)	67 (94%)	4 (6%)	19	20
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	39
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	12
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	61
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	11
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	16
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	16
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	20 (83%)	4 (17%)	2	0
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	12
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	12
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	24
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	35
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	17 (77%)	5 (23%)	1	0
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	36
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	34
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	39
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/138 (85%)	109 (93%)	8 (7%)	14	14
17	v	117/138 (85%)	110 (94%)	7 (6%)	17	18
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	6
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	14
19	Y	19/37 (51%)	18 (95%)	1 (5%)	20	22
19	y	22/37 (60%)	21 (96%)	1 (4%)	24	29
20	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
All	All	4321/4654 (93%)	4134 (96%)	187 (4%)	26	31

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	60	ILE
1	A	205	VAL
1	A	243	GLU
1	A	248	ILE
1	A	270	SER
2	B	84	THR
2	B	86	ILE
2	B	98	LEU
2	B	127	ARG
2	B	236	THR
2	B	240	SER
2	B	282	GLN
2	B	297	THR
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	405	GLU
2	B	409	GLN
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	216	SER
3	C	255	THR
3	C	289	PHE
3	C	315	MET

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Mol	Chain	Res	Type
4	D	43	LEU
4	D	150	ILE
4	D	209	LEU
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	63	LYS
8	I	4	LEU
8	I	6	ILE
10	K	19	ASP
10	K	27	VAL
10	K	43	VAL
12	M	2	GLU
12	M	25	LEU
13	O	6	THR
13	O	34	SER
13	O	39	ARG
13	O	54	GLU
13	O	64	GLU
13	O	78	LEU
13	O	118	LEU
13	O	134	THR
13	O	196	GLN
13	O	214	THR
14	R	6	LEU
14	R	21	ARG
14	R	29	LYS
15	T	25	GLU
16	U	10	VAL
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	28	GLU
17	V	31	ARG
17	V	42	VAL
17	V	86	GLN
17	V	90	GLU
17	V	107	LEU
18	X	3	ILE
18	X	15	LEU

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Mol	Chain	Res	Type
18	X	29	ILE
19	Y	41	VAL
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	19	MET
20	Z	31	GLN
20	Z	32	ASP
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
20	Z	52	LEU
1	a	12	ASN
1	a	42	LEU
1	a	121	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	231	GLU
1	a	245	THR
1	a	288	LEU
2	b	80	ILE
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	246	PHE
2	b	315	ILE
2	b	485	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	165	LEU
3	c	216	SER
3	c	221	GLU

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Mol	Chain	Res	Type
3	c	224	ILE
3	c	240	ILE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
3	c	416	SER
4	d	12	ARG
4	d	90	LEU
4	d	103	ARG
4	d	178	ILE
4	d	182	LEU
4	d	230	SER
4	d	241	GLU
4	d	259	ILE
4	d	264	LYS
4	d	272	LEU
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	39	SER
5	e	65	LEU
5	e	66	VAL
5	e	83	LEU
6	f	25	THR
6	f	28	VAL
7	h	7	LEU
7	h	12	ARG
7	h	30	LEU
7	h	43	LEU
8	i	2	GLU
8	i	6	ILE
9	j	7	ARG
9	j	13	VAL
9	j	21	VAL
9	j	24	ILE
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU

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Mol	Chain	Res	Type
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	143	LYS
13	o	207	ARG
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
14	r	14	LEU
15	t	25	GLU
16	u	51	LYS
17	v	7	VAL
17	v	24	LYS
17	v	52	LEU
17	v	90	GLU
17	v	106	ASN
17	v	107	LEU
17	v	110	LYS
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
20	z	7	LEU
20	z	27	TYR
20	z	32	ASP
20	z	42	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	165	GLN
1	A	315	ASN

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Mol	Chain	Res	Type
1	A	338	ASN
2	B	374	ASN
3	C	327	ASN
4	D	250	ASN
4	D	332	GLN
11	L	8	GLN
12	M	4	ASN
12	M	5	GLN
13	O	36	GLN
13	O	88	ASN
13	O	132	ASN
13	O	196	GLN
16	U	37	GLN
16	U	78	ASN
16	U	81	HIS
17	V	86	GLN
19	Y	45	ASN
20	Z	31	GLN
1	a	12	ASN
1	a	19	ASN
1	a	165	GLN
1	a	181	ASN
2	b	338	GLN
2	b	497	GLN
5	e	60	GLN
5	e	82	GLN
6	f	44	GLN
7	h	59	ASN
12	m	5	GLN
13	o	61	GLN
17	v	118	HIS
20	z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	FME	t	1	15	8,9,10	1.17	1 (12%)	8,9,11	0.89	0
12	FME	M	1	12	8,9,10	1.01	0	8,9,11	1.35	2 (25%)
8	FME	I	1	8	8,9,10	1.05	0	8,9,11	0.74	0
15	FME	T	1	15	8,9,10	0.86	0	8,9,11	1.28	1 (12%)
12	FME	m	1	12	8,9,10	1.12	1 (12%)	8,9,11	0.58	0
8	FME	i	1	8	8,9,10	0.88	0	8,9,11	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	t	1	15	-	2/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.51	1.42	1.46
12	m	1	FME	CA-N	-2.48	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CB-CA-N	2.38	114.85	110.52
12	M	1	FME	CA-N-CN	-2.37	119.18	122.82
15	T	1	FME	C-CA-N	2.03	113.42	109.50

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	i	1	FME	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
15	t	1	FME	O-C-CA-CB
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
8	i	1	FME	CA-CB-CG-SD
8	i	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	i	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 6 are monoatomic - leaving 180 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	c	510	-	69,73,73	1.43	8 (11%)	82,113,113	1.39	10 (12%)
24	BCR	c	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	6 (10%)
30	DGD	h	101	-	63,63,67	1.22	10 (15%)	77,77,81	1.48	14 (18%)
22	CLA	b	615	-	69,73,73	1.57	11 (15%)	82,113,113	1.28	8 (9%)
32	STE	D	412	-	19,19,19	0.65	0	19,19,19	1.21	0
30	DGD	B	623	-	43,43,67	1.24	6 (13%)	45,45,81	1.27	5 (11%)
22	CLA	b	609	-	69,73,73	1.50	10 (14%)	82,113,113	1.48	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	504	36	64,68,73	1.24	9 (14%)	76,107,113	1.25	7 (9%)
22	CLA	c	501	-	69,73,73	1.18	9 (13%)	82,113,113	1.48	8 (9%)
22	CLA	a	411	36	69,73,73	1.29	10 (14%)	82,113,113	1.49	11 (13%)
22	CLA	c	505	-	69,73,73	1.08	7 (10%)	82,113,113	1.29	6 (7%)
32	STE	C	519	-	11,11,19	0.81	0	11,11,19	1.42	2 (18%)
24	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	5 (8%)
32	STE	t	103	-	9,9,19	0.41	0	8,8,19	0.64	0
32	STE	j	101	-	11,11,19	0.99	0	11,11,19	0.86	0
22	CLA	a	405	-	69,73,73	1.42	10 (14%)	82,113,113	1.24	8 (9%)
27	LMG	d	408	-	21,21,55	0.69	1 (4%)	20,20,63	1.05	0
29	SQD	L	101	-	47,49,54	0.95	2 (4%)	57,60,65	2.19	16 (28%)
30	DGD	c	515	-	63,63,67	1.14	7 (11%)	77,77,81	1.37	10 (12%)
27	LMG	a	414	-	49,49,55	0.92	2 (4%)	57,57,63	1.36	5 (8%)
22	CLA	B	614	-	69,73,73	1.43	6 (8%)	82,113,113	1.46	11 (13%)
28	LHG	L	102	-	48,48,48	0.92	2 (4%)	51,54,54	1.18	4 (7%)
24	BCR	B	617	-	41,41,41	1.29	4 (9%)	56,56,56	1.31	8 (14%)
27	LMG	c	520	-	48,48,55	1.10	5 (10%)	56,56,63	1.25	6 (10%)
32	STE	M	103	-	9,9,19	0.40	0	8,8,19	0.74	0
22	CLA	c	512	-	69,73,73	1.29	9 (13%)	82,113,113	1.48	13 (15%)
24	BCR	B	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.12	2 (3%)
27	LMG	A	410	-	48,48,55	0.94	3 (6%)	56,56,63	1.29	5 (8%)
29	SQD	A	412	-	50,52,54	1.06	5 (10%)	60,63,65	1.94	10 (16%)
28	LHG	l	101	-	48,48,48	0.69	0	51,54,54	1.28	5 (9%)
24	BCR	k	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	5 (8%)
22	CLA	B	612	-	69,73,73	1.09	4 (5%)	82,113,113	1.37	10 (12%)
32	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.55	0
22	CLA	c	511	3	69,73,73	1.63	11 (15%)	82,113,113	1.30	4 (4%)
32	STE	x	102	-	19,19,19	0.66	0	19,19,19	1.13	1 (5%)
32	STE	a	415	-	11,11,19	0.96	1 (9%)	11,11,19	0.97	1 (9%)
32	STE	M	102	-	14,14,19	0.75	0	14,14,19	1.16	2 (14%)
22	CLA	B	610	36	69,73,73	1.33	8 (11%)	82,113,113	1.27	8 (9%)
22	CLA	B	616	-	64,68,73	1.31	8 (12%)	76,107,113	1.65	9 (11%)
26	PL9	a	410	-	55,55,55	0.85	2 (3%)	68,69,69	1.74	14 (20%)
22	CLA	b	606	-	69,73,73	1.42	6 (8%)	82,113,113	1.52	5 (6%)
22	CLA	C	510	-	69,73,73	1.36	12 (17%)	82,113,113	1.37	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	619	-	41,41,41	1.23	2 (4%)	56,56,56	1.40	8 (14%)
30	DGD	A	414	-	67,67,67	1.23	8 (11%)	81,81,81	1.32	9 (11%)
32	STE	b	625	-	19,19,19	0.80	1 (5%)	19,19,19	0.87	0
28	LHG	b	623	-	48,48,48	1.02	4 (8%)	51,54,54	1.26	7 (13%)
22	CLA	d	403	-	69,73,73	1.26	10 (14%)	82,113,113	1.13	8 (9%)
32	STE	B	624	-	11,11,19	0.86	0	11,11,19	0.98	0
32	STE	c	519	-	19,19,19	0.61	0	19,19,19	1.21	1 (5%)
22	CLA	C	513	-	69,73,73	1.28	12 (17%)	82,113,113	1.28	10 (12%)
24	BCR	B	619	-	41,41,41	1.32	3 (7%)	56,56,56	1.44	8 (14%)
28	LHG	d	406	-	48,48,48	0.74	1 (2%)	51,54,54	1.27	5 (9%)
22	CLA	B	606	-	69,73,73	1.40	5 (7%)	82,113,113	1.58	7 (8%)
29	SQD	F	102	-	34,36,54	0.95	3 (8%)	42,45,65	2.00	11 (26%)
26	PL9	A	409	-	55,55,55	1.12	2 (3%)	68,69,69	1.66	13 (19%)
22	CLA	b	604	-	69,73,73	1.12	8 (11%)	82,113,113	1.55	9 (10%)
22	CLA	C	507	36	69,73,73	1.12	7 (10%)	82,113,113	1.29	7 (8%)
22	CLA	c	513	-	69,73,73	1.23	10 (14%)	82,113,113	1.23	6 (7%)
24	BCR	C	514	-	41,41,41	1.27	5 (12%)	56,56,56	1.27	4 (7%)
22	CLA	B	609	-	69,73,73	1.21	9 (13%)	82,113,113	1.30	7 (8%)
32	STE	C	521	-	11,11,19	0.62	0	11,11,19	1.40	3 (27%)
31	OEX	a	416	1,36,3	0,15,15	-	-	-	-	-
34	HEM	F	101	5,6	50,50,50	1.43	7 (14%)	67,82,82	1.09	5 (7%)
26	PL9	D	407	-	55,55,55	1.47	8 (14%)	68,69,69	1.69	14 (20%)
22	CLA	C	501	-	69,73,73	1.46	10 (14%)	82,113,113	1.28	9 (10%)
22	CLA	b	601	36	69,73,73	1.42	6 (8%)	82,113,113	1.47	6 (7%)
27	LMG	D	410	-	31,31,55	0.88	1 (3%)	33,33,63	1.20	2 (6%)
28	LHG	E	101	-	48,48,48	0.97	4 (8%)	51,54,54	1.26	8 (15%)
24	BCR	t	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.32	8 (14%)
28	LHG	B	621	-	48,48,48	1.03	3 (6%)	51,54,54	1.35	7 (13%)
32	STE	J	101	-	11,11,19	0.59	0	11,11,19	1.48	2 (18%)
22	CLA	A	405	-	58,62,73	1.63	8 (13%)	68,99,113	1.46	8 (11%)
24	BCR	K	102	-	41,41,41	1.19	3 (7%)	56,56,56	1.28	6 (10%)
35	HEC	V	201	17	46,50,50	1.74	4 (8%)	58,82,82	2.22	11 (18%)
22	CLA	B	604	-	69,73,73	1.33	9 (13%)	82,113,113	1.66	16 (19%)
32	STE	E	102	-	11,11,19	0.86	0	11,11,19	0.97	1 (9%)
33	BCT	a	409	21	3,3,3	1.35	0	2,3,3	3.77	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	c	518	-	37,37,55	0.98	1 (2%)	45,45,63	1.34	7 (15%)
28	LHG	D	409	-	48,48,48	0.81	3 (6%)	51,54,54	1.34	7 (13%)
24	BCR	d	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.20	6 (10%)
29	SQD	a	413	-	35,35,54	1.11	2 (5%)	37,37,65	1.34	4 (10%)
30	DGD	C	515	-	63,63,67	1.26	8 (12%)	77,77,81	1.40	8 (10%)
22	CLA	a	402	-	69,73,73	1.35	11 (15%)	82,113,113	1.24	7 (8%)
32	STE	C	520	-	15,15,19	0.56	0	14,14,19	0.59	0
22	CLA	b	612	-	69,73,73	1.13	6 (8%)	82,113,113	1.27	9 (10%)
22	CLA	C	509	-	69,73,73	1.14	7 (10%)	82,113,113	1.42	10 (12%)
31	OEX	A	415	1,36,3	0,15,15	-	-	-	-	-
22	CLA	C	502	-	69,73,73	1.21	10 (14%)	82,113,113	1.31	11 (13%)
30	DGD	C	516	-	63,63,67	1.24	7 (11%)	77,77,81	1.48	12 (15%)
30	DGD	c	517	-	63,63,67	1.14	6 (9%)	77,77,81	1.50	14 (18%)
22	CLA	B	611	-	69,73,73	1.19	9 (13%)	82,113,113	1.37	11 (13%)
26	PL9	d	405	-	55,55,55	1.46	7 (12%)	68,69,69	1.70	13 (19%)
24	BCR	H	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.36	8 (14%)
32	STE	M	104	-	14,14,19	0.41	0	13,13,19	0.83	0
22	CLA	C	503	-	69,73,73	1.50	8 (11%)	82,113,113	1.73	8 (9%)
22	CLA	b	603	-	69,73,73	1.27	11 (15%)	82,113,113	1.52	12 (14%)
24	BCR	A	406	-	41,41,41	1.07	3 (7%)	56,56,56	1.39	11 (19%)
22	CLA	b	608	-	69,73,73	1.19	7 (10%)	82,113,113	1.09	6 (7%)
29	SQD	a	412	-	52,54,54	0.99	3 (5%)	62,65,65	1.85	13 (20%)
22	CLA	c	503	-	69,73,73	1.28	7 (10%)	82,113,113	1.47	7 (8%)
22	CLA	b	607	36	69,73,73	1.22	10 (14%)	82,113,113	1.32	6 (7%)
22	CLA	C	511	3	69,73,73	1.27	9 (13%)	82,113,113	1.34	9 (10%)
22	CLA	b	613	-	69,73,73	1.17	10 (14%)	82,113,113	1.42	12 (14%)
22	CLA	d	402	-	69,73,73	1.24	6 (8%)	82,113,113	1.36	6 (7%)
22	CLA	B	603	-	69,73,73	1.53	7 (10%)	82,113,113	1.40	17 (20%)
22	CLA	b	616	-	64,68,73	1.22	8 (12%)	76,107,113	1.50	9 (11%)
22	CLA	c	508	-	68,72,73	1.30	12 (17%)	80,111,113	1.41	10 (12%)
32	STE	l	102	-	17,17,19	0.43	0	16,16,19	0.79	0
22	CLA	B	602	-	69,73,73	1.40	9 (13%)	82,113,113	1.31	12 (14%)
24	BCR	Z	101	-	41,41,41	1.14	4 (9%)	56,56,56	1.46	10 (17%)
22	CLA	c	509	-	69,73,73	1.64	9 (13%)	82,113,113	1.28	6 (7%)
30	DGD	C	517	-	63,63,67	1.16	6 (9%)	77,77,81	1.34	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	M	101	-	51,51,55	0.96	3 (5%)	59,59,63	1.36	6 (10%)
22	CLA	B	605	-	69,73,73	1.25	9 (13%)	82,113,113	1.36	8 (9%)
24	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
27	LMG	d	409	-	44,44,55	1.05	4 (9%)	52,52,63	1.36	6 (11%)
22	CLA	c	502	-	69,73,73	1.26	11 (15%)	82,113,113	1.25	11 (13%)
32	STE	b	626	-	9,9,19	0.43	0	8,8,19	0.67	0
24	BCR	D	406	-	41,41,41	1.23	2 (4%)	56,56,56	1.16	5 (8%)
28	LHG	e	102	-	41,41,48	0.94	3 (7%)	44,47,54	1.32	4 (9%)
22	CLA	A	402	-	69,73,73	1.41	7 (10%)	82,113,113	1.27	8 (9%)
22	CLA	b	602	-	69,73,73	1.25	8 (11%)	82,113,113	1.51	11 (13%)
24	BCR	x	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
27	LMG	C	518	-	48,48,55	1.05	6 (12%)	56,56,63	1.37	5 (8%)
27	LMG	D	408	-	51,51,55	0.99	4 (7%)	59,59,63	1.27	6 (10%)
23	PHO	A	404	-	58,69,69	1.79	12 (20%)	55,99,99	1.73	13 (23%)
32	STE	I	101	-	14,14,19	0.54	0	13,13,19	0.58	0
22	CLA	a	403	36	69,73,73	1.26	8 (11%)	82,113,113	1.48	14 (17%)
32	STE	B	625	-	17,17,19	0.76	0	17,17,19	0.95	0
32	STE	t	102	-	13,13,19	0.68	0	13,13,19	1.14	1 (7%)
22	CLA	C	505	-	69,73,73	1.39	10 (14%)	82,113,113	1.33	10 (12%)
32	STE	m	102	-	11,11,19	0.65	0	11,11,19	1.28	1 (9%)
22	CLA	B	615	-	69,73,73	1.30	8 (11%)	82,113,113	1.34	10 (12%)
30	DGD	c	516	-	63,63,67	1.08	5 (7%)	77,77,81	1.39	11 (14%)
27	LMG	D	411	-	26,26,55	0.95	2 (7%)	26,26,63	1.34	3 (11%)
22	CLA	B	608	-	69,73,73	1.46	8 (11%)	82,113,113	1.33	13 (15%)
22	CLA	b	614	-	69,73,73	1.49	11 (15%)	82,113,113	1.34	7 (8%)
35	HEC	v	201	17	46,50,50	1.82	7 (15%)	58,82,82	1.95	8 (13%)
24	BCR	b	617	-	41,41,41	1.24	3 (7%)	56,56,56	1.37	8 (14%)
22	CLA	C	504	36	63,67,73	1.24	9 (14%)	74,105,113	1.24	7 (9%)
32	STE	d	410	-	16,16,19	0.65	0	16,16,19	1.04	0
22	CLA	b	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.47	10 (12%)
32	STE	b	624	-	15,15,19	0.93	1 (6%)	15,15,19	0.73	0
22	CLA	B	607	36	69,73,73	1.26	9 (13%)	82,113,113	1.46	10 (12%)
34	HEM	e	101	5,6	50,50,50	1.43	7 (14%)	67,82,82	1.21	6 (8%)
22	CLA	D	404	36	69,73,73	1.14	4 (5%)	82,113,113	1.30	7 (8%)
27	LMG	m	101	-	51,51,55	1.09	4 (7%)	59,59,63	1.47	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	d	401	-	58,69,69	2.03	11 (18%)	55,99,99	1.52	9 (16%)
24	BCR	b	618	-	41,41,41	1.34	5 (12%)	56,56,56	1.32	10 (17%)
24	BCR	k	103	-	41,41,41	1.04	2 (4%)	56,56,56	1.17	7 (12%)
22	CLA	A	403	36	69,73,73	1.27	10 (14%)	82,113,113	1.19	10 (12%)
28	LHG	d	407	-	38,38,48	0.84	2 (5%)	41,44,54	1.21	2 (4%)
29	SQD	A	413	-	38,38,54	1.06	3 (7%)	40,40,65	1.54	6 (15%)
24	BCR	T	101	-	41,41,41	1.26	5 (12%)	56,56,56	1.34	5 (8%)
33	BCT	D	402	21	3,3,3	1.16	0	2,3,3	2.80	1 (50%)
32	STE	b	620	-	15,15,19	0.56	0	14,14,19	0.70	0
23	PHO	a	404	-	58,69,69	1.97	12 (20%)	55,99,99	1.60	9 (16%)
32	STE	k	104	-	11,11,19	0.96	1 (9%)	11,11,19	1.15	1 (9%)
22	CLA	C	506	-	69,73,73	1.21	7 (10%)	82,113,113	1.15	8 (9%)
22	CLA	b	610	36	69,73,73	1.26	9 (13%)	82,113,113	1.29	10 (12%)
22	CLA	c	507	36	69,73,73	1.40	9 (13%)	82,113,113	1.28	6 (7%)
27	LMG	b	622	-	55,55,55	1.13	6 (10%)	63,63,63	1.46	8 (12%)
29	SQD	B	622	-	52,54,54	0.98	3 (5%)	62,65,65	1.89	13 (20%)
30	DGD	H	102	-	63,63,67	1.43	14 (22%)	77,77,81	1.38	10 (12%)
32	STE	B	627	-	11,11,19	0.78	0	11,11,19	1.09	1 (9%)
22	CLA	C	508	-	69,73,73	1.45	9 (13%)	82,113,113	1.24	9 (10%)
22	CLA	D	405	-	69,73,73	1.67	8 (11%)	82,113,113	1.45	14 (17%)
22	CLA	c	506	-	69,73,73	1.25	9 (13%)	82,113,113	1.19	6 (7%)
24	BCR	a	406	-	41,41,41	1.11	4 (9%)	56,56,56	1.17	2 (3%)
22	CLA	B	601	36	69,73,73	1.62	9 (13%)	82,113,113	1.27	5 (6%)
32	STE	B	626	-	15,15,19	0.47	0	14,14,19	0.72	0
22	CLA	C	512	-	69,73,73	1.27	5 (7%)	82,113,113	1.50	11 (13%)
23	PHO	D	401	-	58,69,69	2.07	12 (20%)	55,99,99	1.41	8 (14%)
32	STE	B	620	-	16,16,19	0.86	1 (6%)	16,16,19	0.87	1 (6%)
22	CLA	B	613	-	69,73,73	1.32	10 (14%)	82,113,113	1.34	9 (10%)
22	CLA	D	403	-	69,73,73	1.23	7 (10%)	82,113,113	1.44	9 (10%)
22	CLA	b	611	-	69,73,73	1.25	8 (11%)	82,113,113	1.43	8 (9%)
28	LHG	A	411	-	46,46,48	1.02	3 (6%)	49,52,54	1.25	3 (6%)
29	SQD	f	101	-	39,41,54	1.13	4 (10%)	49,52,65	1.77	9 (18%)
32	STE	b	621	-	19,19,19	0.68	0	19,19,19	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	510	-	1/1/20/20	9/39/115/115	-
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
30	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	b	615	-	1/1/20/20	9/39/115/115	-
32	STE	D	412	-	-	10/17/17/17	-
30	DGD	B	623	-	-	24/45/45/95	-
22	CLA	b	609	-	1/1/20/20	6/39/115/115	-
22	CLA	c	504	36	1/1/19/20	11/33/109/115	-
22	CLA	c	501	-	1/1/20/20	3/39/115/115	-
22	CLA	a	411	36	1/1/20/20	12/39/115/115	-
22	CLA	c	505	-	1/1/20/20	9/39/115/115	-
32	STE	C	519	-	-	6/9/9/17	-
24	BCR	k	101	-	-	13/29/63/63	0/2/2/2
32	STE	t	103	-	-	4/7/7/17	-
32	STE	j	101	-	-	2/9/9/17	-
22	CLA	a	405	-	1/1/20/20	10/39/115/115	-
27	LMG	d	408	-	-	9/17/17/70	-
29	SQD	L	101	-	-	26/44/64/69	0/1/1/1
30	DGD	c	515	-	-	25/51/91/95	0/2/2/2
27	LMG	a	414	-	-	21/44/64/70	0/1/1/1
22	CLA	B	614	-	1/1/20/20	12/39/115/115	-
28	LHG	L	102	-	-	20/53/53/53	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
27	LMG	c	520	-	-	26/43/63/70	0/1/1/1
32	STE	M	103	-	-	3/7/7/17	-
22	CLA	c	512	-	1/1/20/20	20/39/115/115	-
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2
27	LMG	A	410	-	-	24/43/63/70	0/1/1/1
29	SQD	A	412	-	-	17/47/67/69	0/1/1/1
28	LHG	l	101	-	-	18/53/53/53	-
24	BCR	k	102	-	-	12/29/63/63	0/2/2/2
22	CLA	B	612	-	1/1/20/20	9/39/115/115	-
32	STE	H	103	-	-	10/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	511	3	1/1/20/20	12/39/115/115	-
32	STE	x	102	-	-	13/17/17/17	-
32	STE	a	415	-	-	3/9/9/17	-
32	STE	M	102	-	-	4/12/12/17	-
22	CLA	B	610	36	1/1/20/20	4/39/115/115	-
22	CLA	B	616	-	1/1/19/20	8/33/109/115	-
26	PL9	a	410	-	-	26/53/73/73	0/1/1/1
22	CLA	b	606	-	1/1/20/20	9/39/115/115	-
22	CLA	C	510	-	1/1/20/20	8/39/115/115	-
24	BCR	b	619	-	-	14/29/63/63	0/2/2/2
30	DGD	A	414	-	-	27/55/95/95	0/2/2/2
32	STE	b	625	-	-	5/17/17/17	-
28	LHG	b	623	-	-	24/53/53/53	-
22	CLA	d	403	-	-	5/39/115/115	-
32	STE	B	624	-	-	6/9/9/17	-
32	STE	c	519	-	-	12/17/17/17	-
22	CLA	C	513	-	-	16/39/115/115	-
24	BCR	B	619	-	-	6/29/63/63	0/2/2/2
28	LHG	d	406	-	-	20/53/53/53	-
22	CLA	B	606	-	1/1/20/20	10/39/115/115	-
29	SQD	F	102	-	-	11/28/48/69	0/1/1/1
26	PL9	A	409	-	-	25/53/73/73	0/1/1/1
22	CLA	b	604	-	1/1/20/20	8/39/115/115	-
22	CLA	C	507	36	1/1/20/20	9/39/115/115	-
22	CLA	c	513	-	1/1/20/20	9/39/115/115	-
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
22	CLA	B	609	-	-	4/39/115/115	-
32	STE	C	521	-	-	1/9/9/17	-
34	HEM	F	101	5,6	-	3/14/54/54	-
26	PL9	D	407	-	-	6/53/73/73	0/1/1/1
22	CLA	C	501	-	1/1/20/20	3/39/115/115	-
22	CLA	b	601	36	1/1/20/20	17/39/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
28	LHG	E	101	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	t	101	-	-	8/29/63/63	0/2/2/2
28	LHG	B	621	-	-	16/53/53/53	-
32	STE	J	101	-	-	5/9/9/17	-
22	CLA	A	405	-	1/1/17/20	6/26/102/115	-
24	BCR	K	102	-	-	4/29/63/63	0/2/2/2
35	HEC	V	201	17	-	6/14/54/54	-
22	CLA	B	604	-	1/1/20/20	11/39/115/115	-
32	STE	E	102	-	-	7/9/9/17	-
27	LMG	c	518	-	-	8/31/51/70	0/1/1/1
28	LHG	D	409	-	-	19/53/53/53	-
24	BCR	d	404	-	-	5/29/63/63	0/2/2/2
29	SQD	a	413	-	-	16/37/37/69	-
30	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	a	402	-	1/1/20/20	1/39/115/115	-
32	STE	C	520	-	-	4/13/13/17	-
22	CLA	b	612	-	1/1/20/20	15/39/115/115	-
22	CLA	C	509	-	1/1/20/20	7/39/115/115	-
22	CLA	C	502	-	1/1/20/20	6/39/115/115	-
30	DGD	C	516	-	-	25/51/91/95	0/2/2/2
30	DGD	c	517	-	-	19/51/91/95	0/2/2/2
22	CLA	B	611	-	1/1/20/20	6/39/115/115	-
26	PL9	d	405	-	-	18/53/73/73	0/1/1/1
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
32	STE	M	104	-	-	8/12/12/17	-
22	CLA	C	503	-	1/1/20/20	4/39/115/115	-
22	CLA	b	603	-	1/1/20/20	13/39/115/115	-
24	BCR	A	406	-	-	3/29/63/63	0/2/2/2
22	CLA	b	608	-	-	7/39/115/115	-
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
22	CLA	c	503	-	1/1/20/20	11/39/115/115	-
22	CLA	b	607	36	1/1/20/20	12/39/115/115	-
22	CLA	C	511	3	1/1/20/20	11/39/115/115	-
22	CLA	b	613	-	1/1/20/20	8/39/115/115	-
22	CLA	d	402	-	1/1/20/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	603	-	1/1/20/20	10/39/115/115	-
22	CLA	b	616	-	1/1/19/20	8/33/109/115	-
22	CLA	c	508	-	1/1/19/20	13/38/114/115	-
32	STE	l	102	-	-	13/15/15/17	-
22	CLA	B	602	-	1/1/20/20	9/39/115/115	-
24	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/20/20	16/39/115/115	-
30	DGD	C	517	-	-	12/51/91/95	0/2/2/2
27	LMG	M	101	-	-	27/46/66/70	0/1/1/1
22	CLA	B	605	-	1/1/20/20	10/39/115/115	-
24	BCR	K	101	-	-	11/29/63/63	0/2/2/2
27	LMG	d	409	-	-	12/39/59/70	0/1/1/1
22	CLA	c	502	-	1/1/20/20	15/39/115/115	-
32	STE	b	626	-	-	5/7/7/17	-
24	BCR	D	406	-	-	6/29/63/63	0/2/2/2
28	LHG	e	102	-	-	25/46/46/53	-
22	CLA	A	402	-	1/1/20/20	2/39/115/115	-
22	CLA	b	602	-	1/1/20/20	11/39/115/115	-
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
27	LMG	C	518	-	-	20/43/63/70	0/1/1/1
27	LMG	D	408	-	-	17/46/66/70	0/1/1/1
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
32	STE	I	101	-	-	7/12/12/17	-
22	CLA	a	403	36	1/1/20/20	14/39/115/115	-
32	STE	B	625	-	-	10/15/15/17	-
32	STE	t	102	-	-	3/11/11/17	-
22	CLA	C	505	-	1/1/20/20	10/39/115/115	-
32	STE	m	102	-	-	4/9/9/17	-
22	CLA	B	615	-	1/1/20/20	7/39/115/115	-
30	DGD	c	516	-	-	21/51/91/95	0/2/2/2
27	LMG	D	411	-	-	15/22/22/70	-
22	CLA	B	608	-	-	2/39/115/115	-
22	CLA	b	614	-	1/1/20/20	21/39/115/115	-
35	HEC	v	201	17	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
22	CLA	C	504	36	1/1/18/20	10/32/108/115	-
32	STE	d	410	-	-	7/14/14/17	-
22	CLA	b	605	-	1/1/20/20	9/39/115/115	-
32	STE	b	624	-	-	8/13/13/17	-
22	CLA	B	607	36	1/1/20/20	10/39/115/115	-
34	HEM	e	101	5,6	-	1/14/54/54	-
22	CLA	D	404	36	1/1/20/20	5/39/115/115	-
27	LMG	m	101	-	-	23/46/66/70	0/1/1/1
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
24	BCR	k	103	-	-	8/29/63/63	0/2/2/2
22	CLA	A	403	36	1/1/20/20	5/39/115/115	-
28	LHG	d	407	-	-	14/43/43/53	-
29	SQD	A	413	-	-	13/39/39/69	-
24	BCR	T	101	-	-	11/29/63/63	0/2/2/2
32	STE	b	620	-	-	7/13/13/17	-
23	PHO	a	404	-	-	6/37/103/103	0/5/6/6
32	STE	k	104	-	-	2/9/9/17	-
22	CLA	C	506	-	1/1/20/20	12/39/115/115	-
22	CLA	b	610	36	1/1/20/20	7/39/115/115	-
22	CLA	c	507	36	1/1/20/20	12/39/115/115	-
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
29	SQD	B	622	-	-	16/49/69/69	0/1/1/1
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
32	STE	B	627	-	-	7/9/9/17	-
22	CLA	C	508	-	-	5/39/115/115	-
22	CLA	D	405	-	-	9/39/115/115	-
22	CLA	c	506	-	1/1/20/20	13/39/115/115	-
24	BCR	a	406	-	-	5/29/63/63	0/2/2/2
22	CLA	B	601	36	1/1/20/20	19/39/115/115	-
32	STE	B	626	-	-	6/13/13/17	-
22	CLA	C	512	-	1/1/20/20	21/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
32	STE	B	620	-	-	8/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	613	-	1/1/20/20	14/39/115/115	-
22	CLA	D	403	-	1/1/20/20	7/39/115/115	-
22	CLA	b	611	-	1/1/20/20	10/39/115/115	-
28	LHG	A	411	-	-	22/51/51/53	-
29	SQD	f	101	-	-	12/36/56/69	0/1/1/1
32	STE	b	621	-	-	9/17/17/17	-

All (930) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C1B-C2B	8.96	1.49	1.39
22	D	405	CLA	MG-NB	-8.64	1.88	2.05
23	D	401	PHO	C3B-C4B	8.45	1.50	1.41
23	D	401	PHO	C1B-C2B	8.45	1.48	1.39
23	a	404	PHO	C1B-C2B	8.38	1.48	1.39
22	c	509	CLA	MG-NB	-8.01	1.89	2.05
23	d	401	PHO	C3B-C4B	8.00	1.49	1.41
23	a	404	PHO	C3B-C4B	7.66	1.49	1.41
22	b	606	CLA	MG-NA	7.43	2.23	2.06
22	C	503	CLA	MG-NA	7.39	2.23	2.06
22	B	606	CLA	MG-NA	7.31	2.23	2.06
22	B	601	CLA	MG-NA	6.99	2.22	2.06
22	A	405	CLA	MG-NB	-6.85	1.92	2.05
22	B	614	CLA	MG-ND	-6.74	1.92	2.05
23	A	404	PHO	C1B-C2B	6.64	1.46	1.39
26	D	407	PL9	C7-C3	-6.54	1.42	1.51
22	b	601	CLA	MG-NA	6.53	2.21	2.06
22	D	405	CLA	MG-NC	6.43	2.21	2.06
22	b	615	CLA	MG-NA	6.39	2.21	2.06
35	V	201	HEC	CAC-C3C	6.39	1.55	1.35
22	A	402	CLA	MG-NB	6.33	2.18	2.05
35	v	201	HEC	CAC-C3C	6.30	1.55	1.35
22	B	608	CLA	MG-NA	6.30	2.21	2.06
35	V	201	HEC	CAB-C3B	6.16	1.55	1.35
23	A	404	PHO	C3B-C4B	6.14	1.47	1.41
22	C	508	CLA	MG-NA	6.12	2.20	2.06
35	v	201	HEC	CAB-C3B	6.02	1.54	1.35
22	c	511	CLA	MG-NA	5.88	2.20	2.06
22	B	603	CLA	MG-ND	5.83	2.17	2.05
22	B	603	CLA	MG-NB	-5.72	1.94	2.05
22	B	613	CLA	MG-ND	-5.58	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	MG-ND	-5.58	1.94	2.05
22	B	601	CLA	MG-NB	-5.56	1.94	2.05
26	d	405	PL9	C6-C1	-5.54	1.39	1.48
22	c	510	CLA	MG-NA	5.38	2.19	2.06
22	C	501	CLA	MG-NB	-5.37	1.95	2.05
22	c	509	CLA	MG-ND	5.37	2.16	2.05
22	a	405	CLA	MG-NC	-5.27	1.93	2.06
22	C	510	CLA	MG-NC	5.22	2.18	2.06
22	b	615	CLA	MG-NC	-5.17	1.94	2.06
22	C	505	CLA	MG-NC	5.17	2.18	2.06
22	b	609	CLA	MG-ND	-5.15	1.95	2.05
22	b	614	CLA	MG-ND	-4.98	1.95	2.05
35	v	201	HEC	C3D-C2D	4.90	1.51	1.38
22	c	507	CLA	MG-NA	4.86	2.17	2.06
22	c	503	CLA	MG-NC	4.85	2.17	2.06
22	c	510	CLA	MG-ND	-4.72	1.96	2.05
22	c	507	CLA	MG-NB	-4.70	1.96	2.05
22	C	505	CLA	MG-NB	-4.69	1.96	2.05
24	b	618	BCR	C30-C25	-4.66	1.47	1.53
24	H	101	BCR	C30-C25	-4.63	1.47	1.53
22	c	511	CLA	MG-NB	-4.55	1.96	2.05
22	B	608	CLA	MG-ND	-4.49	1.96	2.05
22	C	512	CLA	MG-NA	4.48	2.16	2.06
24	B	617	BCR	C30-C25	-4.48	1.48	1.53
24	T	101	BCR	C30-C25	-4.47	1.48	1.53
22	B	603	CLA	MG-NA	4.47	2.16	2.06
22	C	512	CLA	MG-NB	4.46	2.14	2.05
24	B	619	BCR	C30-C25	-4.46	1.48	1.53
24	b	617	BCR	C1-C6	-4.46	1.48	1.53
22	c	508	CLA	MG-NB	4.41	2.14	2.05
22	b	603	CLA	MG-NA	4.39	2.16	2.06
22	B	605	CLA	C1D-ND	4.36	1.43	1.37
22	C	501	CLA	MG-NA	4.31	2.16	2.06
22	b	602	CLA	MG-NA	4.26	2.16	2.06
24	b	619	BCR	C30-C25	-4.23	1.48	1.53
24	B	619	BCR	C1-C6	-4.22	1.48	1.53
24	K	102	BCR	C30-C25	-4.22	1.48	1.53
22	c	511	CLA	MG-ND	4.21	2.14	2.05
22	C	511	CLA	MG-NA	4.12	2.16	2.06
35	V	201	HEC	C3D-C2D	4.11	1.49	1.38
22	C	503	CLA	MG-NB	4.09	2.13	2.05
22	b	614	CLA	C1D-ND	4.08	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	MG-NA	4.07	2.15	2.06
30	C	517	DGD	O2G-C2G	-4.06	1.37	1.46
24	D	406	BCR	C30-C25	-4.04	1.48	1.53
24	C	514	BCR	C1-C6	-4.04	1.48	1.53
24	B	617	BCR	C1-C6	-4.03	1.48	1.53
27	m	101	LMG	C4-C3	4.03	1.62	1.52
22	a	411	CLA	MG-NA	4.01	2.15	2.06
29	a	413	SQD	O47-C7	4.01	1.45	1.34
22	b	609	CLA	C1D-ND	4.00	1.43	1.37
22	b	609	CLA	MG-NC	4.00	2.15	2.06
22	c	512	CLA	MG-NB	3.98	2.13	2.05
23	D	401	PHO	C4D-ND	-3.98	1.32	1.38
22	c	511	CLA	C1D-ND	3.94	1.43	1.37
22	a	403	CLA	MG-NC	3.93	2.15	2.06
24	d	404	BCR	C1-C6	-3.90	1.48	1.53
22	b	614	CLA	MG-NB	3.89	2.13	2.05
28	b	623	LHG	O7-C5	-3.89	1.37	1.46
26	A	409	PL9	C7-C3	-3.89	1.46	1.51
26	A	409	PL9	C3-C4	-3.86	1.43	1.49
28	A	411	LHG	P-O6	3.86	1.74	1.59
22	C	513	CLA	MG-NA	3.86	2.15	2.06
34	e	101	HEM	FE-NA	3.85	2.07	1.95
24	t	101	BCR	C1-C6	-3.83	1.48	1.53
24	C	514	BCR	C30-C25	-3.82	1.48	1.53
26	d	405	PL9	C53-C6	-3.80	1.43	1.50
22	B	607	CLA	MG-NC	3.79	2.15	2.06
22	c	513	CLA	MG-ND	-3.79	1.98	2.05
22	D	403	CLA	MG-NA	3.79	2.15	2.06
22	c	502	CLA	MG-NB	-3.78	1.98	2.05
22	B	601	CLA	C4B-NB	3.77	1.42	1.37
22	b	611	CLA	MG-NA	3.76	2.15	2.06
24	t	101	BCR	C30-C25	-3.76	1.49	1.53
24	x	101	BCR	C30-C25	-3.76	1.49	1.53
22	b	614	CLA	MG-NA	3.75	2.15	2.06
22	b	606	CLA	C1D-ND	3.72	1.42	1.37
22	d	402	CLA	C1D-ND	3.71	1.42	1.37
22	B	602	CLA	MG-NB	3.71	2.13	2.05
22	B	610	CLA	MG-ND	-3.71	1.98	2.05
22	c	510	CLA	C1D-ND	3.70	1.42	1.37
29	L	101	SQD	O48-C23	3.70	1.44	1.33
22	A	405	CLA	MG-NC	3.70	2.15	2.06
22	b	609	CLA	C4B-NB	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	402	CLA	C1D-ND	3.68	1.42	1.37
29	A	413	SQD	O47-C7	3.68	1.44	1.34
27	b	622	LMG	O6-C1	3.66	1.51	1.41
29	a	412	SQD	O48-C23	3.64	1.44	1.33
24	K	101	BCR	C30-C25	-3.63	1.49	1.53
29	B	622	SQD	O47-C7	3.63	1.44	1.34
22	B	615	CLA	C1D-ND	3.63	1.42	1.37
24	k	101	BCR	C30-C25	-3.62	1.49	1.53
28	B	621	LHG	O7-C5	-3.61	1.38	1.46
22	C	510	CLA	C1D-ND	3.58	1.42	1.37
30	B	623	DGD	O1G-C1A	3.57	1.43	1.33
22	D	403	CLA	CMB-C2B	-3.57	1.43	1.50
22	b	610	CLA	MG-NB	-3.57	1.98	2.05
24	D	406	BCR	C1-C6	-3.56	1.49	1.53
22	A	405	CLA	C1D-ND	3.55	1.42	1.37
22	c	504	CLA	C4B-NB	3.54	1.42	1.37
22	C	508	CLA	C4B-NB	3.53	1.42	1.37
22	B	610	CLA	C1D-ND	3.53	1.42	1.37
24	B	618	BCR	C30-C25	-3.53	1.49	1.53
22	B	601	CLA	C1D-ND	3.51	1.42	1.37
22	d	402	CLA	MG-NA	3.51	2.14	2.06
22	b	602	CLA	C1D-ND	3.51	1.42	1.37
22	B	615	CLA	MG-NA	3.50	2.14	2.06
34	e	101	HEM	FE-NB	3.50	2.05	1.94
30	C	516	DGD	C4D-C3D	3.50	1.61	1.52
22	a	405	CLA	C1D-ND	3.49	1.42	1.37
22	d	403	CLA	C1D-ND	3.48	1.42	1.37
22	a	405	CLA	MG-NA	3.44	2.14	2.06
22	C	501	CLA	C1B-NB	-3.44	1.33	1.37
27	M	101	LMG	C9-C8	3.44	1.61	1.50
22	b	609	CLA	CMB-C2B	-3.43	1.43	1.50
22	b	610	CLA	C1D-ND	3.43	1.42	1.37
30	H	102	DGD	O5D-C1E	3.43	1.45	1.40
22	B	613	CLA	C1B-NB	-3.43	1.33	1.37
24	b	619	BCR	C1-C6	-3.43	1.49	1.53
22	D	403	CLA	CMD-C2D	-3.41	1.43	1.50
22	b	608	CLA	C1B-C2B	3.41	1.51	1.43
22	B	616	CLA	MG-NA	3.41	2.14	2.06
22	B	614	CLA	MG-NA	3.40	2.14	2.06
24	Z	101	BCR	C1-C6	-3.40	1.49	1.53
22	B	616	CLA	C1D-ND	3.40	1.42	1.37
22	b	611	CLA	C4B-NB	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	515	DGD	C4D-C3D	3.39	1.61	1.52
30	A	414	DGD	C4E-C5E	3.39	1.60	1.53
24	k	102	BCR	C1-C6	-3.39	1.49	1.53
22	B	609	CLA	C1B-C2B	3.38	1.51	1.43
30	H	102	DGD	O5D-C6D	-3.38	1.37	1.43
30	C	516	DGD	O3D-C3D	-3.37	1.34	1.43
22	B	610	CLA	CMB-C2B	-3.37	1.43	1.50
29	f	101	SQD	O47-C7	3.36	1.43	1.34
22	A	403	CLA	CMD-C2D	-3.34	1.43	1.50
22	a	402	CLA	MG-NA	3.34	2.14	2.06
22	b	605	CLA	MG-NA	3.34	2.14	2.06
34	F	101	HEM	FE-NA	3.32	2.06	1.95
22	B	614	CLA	C4B-NB	3.32	1.42	1.37
23	d	401	PHO	C1D-C2D	3.32	1.43	1.39
22	a	403	CLA	C4B-NB	3.32	1.42	1.37
23	A	404	PHO	CMD-C2D	-3.32	1.45	1.51
22	c	509	CLA	C1B-C2B	3.30	1.50	1.43
29	f	101	SQD	O48-C23	3.29	1.43	1.33
22	b	601	CLA	C1B-C2B	3.29	1.50	1.43
22	c	511	CLA	C4B-NB	3.29	1.42	1.37
22	A	403	CLA	C1D-ND	3.29	1.42	1.37
28	E	101	LHG	P-O6	3.28	1.72	1.59
30	c	515	DGD	O2G-C2G	-3.28	1.38	1.46
22	B	611	CLA	MG-NA	3.28	2.14	2.06
34	F	101	HEM	FE-NC	3.28	2.06	1.95
24	K	101	BCR	C1-C6	-3.28	1.49	1.53
23	a	404	PHO	C1D-C2D	3.26	1.43	1.39
22	c	512	CLA	C1D-ND	3.26	1.42	1.37
22	B	608	CLA	C1D-ND	3.25	1.42	1.37
22	b	616	CLA	C1D-ND	3.25	1.42	1.37
23	D	401	PHO	C3B-C2B	-3.24	1.36	1.40
24	d	404	BCR	C30-C25	-3.24	1.49	1.53
22	b	615	CLA	MG-NB	3.23	2.12	2.05
22	A	405	CLA	C1B-NB	-3.23	1.33	1.37
24	Z	101	BCR	C30-C25	-3.23	1.49	1.53
30	C	515	DGD	C6E-C5E	3.23	1.62	1.51
22	B	610	CLA	C4B-NB	3.22	1.42	1.37
30	c	516	DGD	O2E-C2E	-3.22	1.35	1.43
24	c	514	BCR	C1-C6	-3.22	1.49	1.53
22	C	513	CLA	C1D-ND	3.21	1.42	1.37
22	D	405	CLA	C1D-ND	3.20	1.42	1.37
24	b	617	BCR	C30-C25	-3.20	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	622	LMG	C3-C2	3.19	1.60	1.52
22	C	505	CLA	C4B-NB	3.18	1.42	1.37
24	c	514	BCR	C30-C25	-3.17	1.49	1.53
22	B	604	CLA	MG-ND	-3.17	1.99	2.05
23	d	401	PHO	CMC-C2C	-3.16	1.45	1.50
27	D	411	LMG	O8-C28	3.15	1.41	1.30
27	d	409	LMG	C4-C5	3.15	1.59	1.53
23	D	401	PHO	CMB-C2B	-3.15	1.45	1.51
22	c	506	CLA	MG-ND	-3.14	1.99	2.05
22	B	604	CLA	C3B-C4B	3.14	1.51	1.42
22	B	601	CLA	C1B-C2B	3.14	1.50	1.43
22	B	604	CLA	C1B-C2B	3.13	1.50	1.43
30	c	515	DGD	O5D-C1E	3.13	1.45	1.40
22	b	616	CLA	MG-NA	3.12	2.13	2.06
24	k	102	BCR	C30-C25	-3.12	1.49	1.53
30	c	517	DGD	O2G-C2G	-3.12	1.39	1.46
23	A	404	PHO	C3B-C2B	-3.11	1.36	1.40
24	A	406	BCR	C1-C6	-3.10	1.49	1.53
22	B	616	CLA	MG-ND	3.10	2.11	2.05
22	a	403	CLA	CHC-C1C	3.10	1.44	1.38
22	a	411	CLA	C1D-ND	3.10	1.41	1.37
30	C	517	DGD	O1G-C1G	-3.09	1.38	1.45
22	A	402	CLA	C1B-C2B	3.09	1.50	1.43
22	C	510	CLA	C1B-NB	-3.09	1.33	1.37
29	A	413	SQD	O48-C23	3.08	1.42	1.33
22	B	614	CLA	C1D-ND	3.06	1.41	1.37
29	L	101	SQD	O47-C7	3.06	1.42	1.34
22	D	404	CLA	C1D-ND	3.06	1.41	1.37
27	m	101	LMG	C4-C5	3.06	1.59	1.53
22	a	405	CLA	C1B-C2B	3.06	1.50	1.43
22	B	607	CLA	MG-NB	-3.04	1.99	2.05
22	c	513	CLA	C1D-ND	3.04	1.41	1.37
22	C	507	CLA	C4B-NB	3.03	1.41	1.37
22	c	503	CLA	C1D-ND	3.03	1.41	1.37
22	A	403	CLA	C1B-C2B	3.03	1.50	1.43
22	B	611	CLA	CMD-C2D	-3.03	1.44	1.50
22	C	506	CLA	MG-NB	-3.03	1.99	2.05
22	A	405	CLA	MG-NA	-3.03	1.99	2.06
29	A	412	SQD	O47-C7	3.03	1.42	1.34
22	c	505	CLA	C1B-C2B	3.02	1.50	1.43
22	c	511	CLA	MG-NC	3.02	2.13	2.06
30	A	414	DGD	C3G-C2G	3.01	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	102	SQD	O48-C23	3.01	1.42	1.33
22	c	506	CLA	C1D-ND	3.01	1.41	1.37
22	c	501	CLA	MG-NB	-3.01	1.99	2.05
22	B	605	CLA	C1B-C2B	3.01	1.50	1.43
22	b	601	CLA	C1D-ND	3.00	1.41	1.37
22	B	603	CLA	C1D-ND	2.99	1.41	1.37
27	D	408	LMG	O2-C2	-2.99	1.35	1.43
22	a	402	CLA	C1B-C2B	2.99	1.50	1.43
22	c	502	CLA	CMD-C2D	-2.98	1.44	1.50
22	C	504	CLA	C1D-ND	2.98	1.41	1.37
30	H	102	DGD	O2G-C2G	-2.98	1.39	1.46
24	B	618	BCR	C1-C6	-2.98	1.50	1.53
22	c	512	CLA	C4B-NB	2.98	1.41	1.37
22	C	507	CLA	C1B-C2B	2.97	1.50	1.43
29	A	412	SQD	O2-C2	-2.97	1.35	1.43
22	c	510	CLA	CMB-C2B	-2.97	1.44	1.50
22	C	505	CLA	CHC-C1C	2.97	1.44	1.38
22	C	501	CLA	C4B-NB	2.97	1.41	1.37
22	B	612	CLA	MG-NA	2.96	2.13	2.06
29	B	622	SQD	O48-C23	2.96	1.42	1.33
22	B	609	CLA	C1D-ND	2.95	1.41	1.37
30	B	623	DGD	C1G-C2G	2.95	1.60	1.50
22	c	507	CLA	MG-NC	-2.94	1.99	2.06
22	a	402	CLA	MG-ND	-2.94	2.00	2.05
22	d	403	CLA	C4B-NB	2.94	1.41	1.37
22	b	601	CLA	C4B-NB	2.94	1.41	1.37
29	a	413	SQD	O48-C23	2.93	1.41	1.33
22	D	404	CLA	C1B-NB	-2.93	1.34	1.37
30	c	516	DGD	O3E-C3E	-2.93	1.35	1.43
27	A	410	LMG	C4-C3	2.93	1.59	1.52
26	d	405	PL9	C31-C29	-2.93	1.45	1.51
22	b	607	CLA	CMB-C2B	-2.93	1.44	1.50
22	C	508	CLA	C1B-C2B	2.93	1.50	1.43
27	C	518	LMG	C1-C2	2.93	1.61	1.52
24	a	406	BCR	C1-C6	-2.93	1.50	1.53
30	H	102	DGD	O4D-C4D	-2.92	1.35	1.43
22	C	503	CLA	C1B-C2B	2.92	1.50	1.43
22	c	501	CLA	MG-NA	2.92	2.13	2.06
22	C	501	CLA	CMD-C2D	-2.91	1.44	1.50
27	C	518	LMG	C4-C5	2.91	1.59	1.53
26	D	407	PL9	C11-C9	-2.91	1.45	1.51
22	a	403	CLA	C1D-ND	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	410	LMG	C7-C8	2.90	1.58	1.51
22	b	602	CLA	C4B-NB	2.90	1.41	1.37
27	M	101	LMG	O7-C8	-2.90	1.39	1.46
22	B	616	CLA	CMD-C2D	-2.89	1.44	1.50
22	a	405	CLA	MG-ND	-2.89	2.00	2.05
28	L	102	LHG	O8-C23	2.89	1.41	1.33
22	C	502	CLA	MG-NC	2.89	2.13	2.06
22	b	607	CLA	MG-ND	-2.89	2.00	2.05
28	e	102	LHG	P-O6	2.89	1.70	1.59
22	B	610	CLA	MG-NA	2.89	2.13	2.06
22	d	403	CLA	MG-ND	-2.89	2.00	2.05
22	B	610	CLA	MG-NB	-2.88	2.00	2.05
22	b	603	CLA	C3B-C4B	2.88	1.51	1.42
27	c	520	LMG	C7-C8	2.88	1.59	1.50
22	C	506	CLA	C4B-NB	2.87	1.41	1.37
22	b	611	CLA	C1B-NB	-2.87	1.34	1.37
22	b	611	CLA	C1B-C2B	2.87	1.49	1.43
22	c	512	CLA	C3B-C4B	2.86	1.51	1.42
22	C	501	CLA	C1D-ND	2.86	1.41	1.37
30	C	516	DGD	C6D-C5D	2.86	1.60	1.51
23	A	404	PHO	C1D-C2D	2.86	1.42	1.39
22	A	405	CLA	C4B-NB	2.86	1.41	1.37
22	b	615	CLA	CMB-C2B	-2.85	1.44	1.50
22	C	505	CLA	C1B-C2B	2.84	1.49	1.43
22	C	508	CLA	MG-ND	-2.84	2.00	2.05
22	B	609	CLA	MG-NB	-2.83	2.00	2.05
22	b	605	CLA	C3B-C4B	2.83	1.51	1.42
22	a	402	CLA	C3B-C4B	2.83	1.51	1.42
30	B	623	DGD	O2G-C2G	-2.83	1.39	1.46
22	c	506	CLA	MG-NC	2.83	2.13	2.06
22	C	509	CLA	C1D-ND	2.83	1.41	1.37
29	A	413	SQD	O47-C45	-2.82	1.42	1.47
30	c	516	DGD	O5D-C1E	2.82	1.44	1.40
22	B	606	CLA	C1D-ND	2.82	1.41	1.37
22	B	615	CLA	C4B-NB	2.82	1.41	1.37
22	b	602	CLA	C1B-C2B	2.82	1.49	1.43
30	h	101	DGD	C3G-C2G	2.81	1.59	1.50
23	A	404	PHO	CMC-C2C	-2.81	1.46	1.50
22	a	403	CLA	C1B-NB	-2.80	1.34	1.37
22	A	402	CLA	C1B-NB	-2.80	1.34	1.37
22	C	504	CLA	C1B-NB	-2.79	1.34	1.37
30	A	414	DGD	C3E-C2E	2.79	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	103	BCR	C30-C25	-2.79	1.50	1.53
22	B	609	CLA	CMD-C2D	-2.79	1.45	1.50
22	b	613	CLA	MG-NC	-2.78	1.99	2.06
22	d	403	CLA	CMD-C2D	-2.78	1.45	1.50
22	a	411	CLA	CHC-C1C	2.78	1.44	1.38
22	B	610	CLA	C3B-C4B	2.78	1.50	1.42
22	d	402	CLA	CMB-C2B	-2.77	1.45	1.50
27	d	409	LMG	O6-C5	-2.77	1.37	1.44
22	c	503	CLA	C4B-NB	2.77	1.41	1.37
22	B	603	CLA	CMC-C2C	-2.77	1.45	1.50
22	c	506	CLA	C4B-NB	2.77	1.41	1.37
22	B	611	CLA	C1B-NB	-2.77	1.34	1.37
22	C	511	CLA	C1D-ND	2.76	1.41	1.37
23	a	404	PHO	CAC-C3C	-2.76	1.46	1.51
23	D	401	PHO	CMD-C2D	-2.76	1.46	1.51
22	C	511	CLA	MG-NC	2.76	2.12	2.06
22	B	602	CLA	CMD-C2D	-2.76	1.45	1.50
30	C	515	DGD	O2G-C2G	-2.76	1.40	1.46
22	C	511	CLA	C1B-C2B	2.75	1.49	1.43
23	d	401	PHO	C4D-ND	-2.75	1.34	1.38
22	c	512	CLA	C1B-C2B	2.75	1.49	1.43
24	a	406	BCR	C38-C26	-2.74	1.46	1.50
22	c	511	CLA	C1B-C2B	2.74	1.49	1.43
22	C	513	CLA	MG-ND	2.74	2.11	2.05
22	C	509	CLA	CMB-C2B	-2.74	1.45	1.50
23	d	401	PHO	CMD-C2D	-2.74	1.46	1.51
22	b	604	CLA	C4B-NB	2.73	1.41	1.37
30	h	101	DGD	O3E-C3E	-2.73	1.36	1.43
22	b	612	CLA	C1B-C2B	2.73	1.49	1.43
22	C	510	CLA	CHC-C1C	2.73	1.43	1.38
22	c	512	CLA	CMB-C2B	-2.72	1.45	1.50
22	c	501	CLA	C1B-C2B	2.72	1.49	1.43
22	c	507	CLA	C1B-C2B	2.72	1.49	1.43
22	b	602	CLA	CMD-C2D	-2.71	1.45	1.50
22	c	507	CLA	MG-ND	2.71	2.11	2.05
22	B	616	CLA	CMC-C2C	-2.71	1.45	1.50
22	a	402	CLA	C4B-NB	2.71	1.41	1.37
24	K	102	BCR	C1-C6	-2.71	1.50	1.53
22	A	403	CLA	MG-NC	2.71	2.12	2.06
22	B	607	CLA	C1D-ND	2.70	1.41	1.37
28	A	411	LHG	O3-C3	-2.70	1.34	1.44
23	a	404	PHO	CBD-CGD	-2.70	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	C1B-C2B	2.70	1.49	1.43
22	B	612	CLA	CMC-C2C	-2.69	1.45	1.50
22	a	405	CLA	CMC-C2C	-2.69	1.45	1.50
30	B	623	DGD	O2G-C1B	2.69	1.41	1.34
22	b	610	CLA	CMD-C2D	-2.69	1.45	1.50
34	F	101	HEM	CAC-C3C	2.68	1.54	1.47
22	b	613	CLA	MG-NA	2.68	2.12	2.06
22	B	615	CLA	CMB-C2B	-2.68	1.45	1.50
22	c	513	CLA	C4B-NB	2.68	1.41	1.37
22	C	507	CLA	MG-NB	-2.68	2.00	2.05
22	a	405	CLA	CMD-C2D	-2.68	1.45	1.50
22	c	503	CLA	CMC-C2C	-2.68	1.45	1.50
22	B	614	CLA	CMB-C2B	-2.67	1.45	1.50
22	C	502	CLA	CMD-C2D	-2.67	1.45	1.50
23	A	404	PHO	C4D-ND	-2.67	1.34	1.38
22	b	612	CLA	C3B-C4B	2.67	1.50	1.42
27	c	520	LMG	C3-C2	2.66	1.59	1.52
26	d	405	PL9	C10-C9	-2.66	1.44	1.50
22	C	513	CLA	C1B-C2B	2.66	1.49	1.43
26	D	407	PL9	C52-C5	-2.66	1.45	1.50
29	A	412	SQD	O48-C23	2.66	1.41	1.33
22	c	509	CLA	C4B-NB	2.66	1.41	1.37
22	b	615	CLA	CMC-C2C	-2.66	1.45	1.50
22	C	511	CLA	C3B-C4B	2.66	1.50	1.42
27	D	408	LMG	C4-C5	2.65	1.58	1.53
30	H	102	DGD	C4D-C5D	2.65	1.58	1.53
22	c	505	CLA	CMB-C2B	-2.65	1.45	1.50
22	a	411	CLA	CHD-C4C	2.65	1.45	1.39
22	B	604	CLA	MG-NC	2.65	2.12	2.06
22	A	403	CLA	C4B-NB	2.65	1.41	1.37
30	c	517	DGD	O5D-C1E	2.65	1.44	1.40
22	C	511	CLA	CMB-C2B	-2.65	1.45	1.50
22	a	411	CLA	C4B-NB	2.65	1.41	1.37
22	c	504	CLA	C1D-ND	2.65	1.41	1.37
30	C	517	DGD	O6D-C5D	-2.64	1.37	1.44
22	B	604	CLA	MG-NB	2.64	2.11	2.05
22	B	602	CLA	C4B-NB	2.64	1.41	1.37
22	b	615	CLA	CMD-C2D	-2.64	1.45	1.50
22	C	506	CLA	C1B-C2B	2.63	1.49	1.43
22	b	604	CLA	CMC-C2C	-2.63	1.45	1.50
22	b	603	CLA	C1D-ND	2.63	1.41	1.37
30	h	101	DGD	C4E-C5E	2.63	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	402	CLA	CMC-C2C	-2.63	1.45	1.50
24	k	101	BCR	C1-C6	-2.63	1.50	1.53
22	c	508	CLA	MG-NC	2.63	2.12	2.06
22	C	504	CLA	C4B-NB	2.62	1.41	1.37
22	B	615	CLA	MG-NB	2.62	2.11	2.05
22	b	613	CLA	CMD-C2D	-2.62	1.45	1.50
22	b	616	CLA	CMD-C2D	-2.62	1.45	1.50
22	A	402	CLA	C3B-C4B	2.62	1.50	1.42
22	C	508	CLA	CHC-C1C	2.61	1.43	1.38
22	b	613	CLA	CMB-C2B	-2.61	1.45	1.50
30	A	414	DGD	C6E-C5E	2.61	1.60	1.51
23	a	404	PHO	CMB-C2B	-2.61	1.46	1.51
30	A	414	DGD	C4D-C3D	2.60	1.59	1.52
22	C	504	CLA	C1B-C2B	2.60	1.49	1.43
22	b	614	CLA	CHC-C1C	2.60	1.43	1.38
22	d	402	CLA	C1B-C2B	2.60	1.49	1.43
27	d	409	LMG	O7-C8	-2.59	1.40	1.46
22	d	403	CLA	CMB-C2B	-2.59	1.45	1.50
22	B	611	CLA	C1B-C2B	2.59	1.49	1.43
22	B	613	CLA	C4B-NB	2.59	1.41	1.37
26	a	410	PL9	C53-C6	-2.59	1.45	1.50
22	b	604	CLA	C1B-C2B	2.59	1.49	1.43
24	a	406	BCR	C30-C25	-2.59	1.50	1.53
22	C	508	CLA	C1D-ND	2.59	1.41	1.37
30	H	102	DGD	C1E-C2E	2.59	1.60	1.52
22	B	607	CLA	CMD-C2D	-2.58	1.45	1.50
22	c	504	CLA	C1B-C2B	2.58	1.49	1.43
22	C	501	CLA	CMC-C2C	-2.58	1.45	1.50
27	m	101	LMG	O6-C1	2.58	1.48	1.41
22	b	608	CLA	C4B-NB	2.58	1.41	1.37
22	C	513	CLA	CMB-C2B	-2.57	1.45	1.50
22	b	608	CLA	C1B-NB	-2.57	1.34	1.37
22	c	502	CLA	C3B-C4B	2.57	1.50	1.42
22	b	612	CLA	CMB-C2B	-2.57	1.45	1.50
22	c	509	CLA	C3B-C4B	2.57	1.50	1.42
22	a	402	CLA	CMB-C2B	-2.57	1.45	1.50
22	B	606	CLA	CHC-C1C	2.57	1.43	1.38
22	D	405	CLA	CMB-C2B	-2.56	1.45	1.50
24	x	101	BCR	C1-C6	-2.56	1.50	1.53
28	b	623	LHG	P-O6	2.56	1.69	1.59
22	c	511	CLA	CHC-C1C	2.56	1.43	1.38
22	C	502	CLA	MG-ND	-2.56	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	CMD-C2D	-2.56	1.45	1.50
22	B	615	CLA	MG-ND	-2.56	2.00	2.05
22	c	505	CLA	C3B-C4B	2.56	1.50	1.42
22	c	508	CLA	MG-NA	2.55	2.12	2.06
30	H	102	DGD	C6E-C5E	2.55	1.60	1.51
22	b	605	CLA	MG-NB	2.55	2.10	2.05
22	D	403	CLA	C1B-C2B	2.54	1.49	1.43
22	b	616	CLA	MG-ND	-2.54	2.00	2.05
22	b	604	CLA	MG-NA	2.54	2.12	2.06
22	c	502	CLA	MG-ND	2.54	2.10	2.05
22	c	504	CLA	C3B-C4B	2.54	1.50	1.42
22	b	602	CLA	CMC-C2C	-2.54	1.45	1.50
22	c	505	CLA	C4B-NB	2.54	1.41	1.37
34	e	101	HEM	C3B-C2B	-2.54	1.32	1.37
27	D	411	LMG	C29-C28	2.54	1.56	1.50
27	M	101	LMG	C3-C2	2.54	1.58	1.52
22	C	511	CLA	C4B-NB	2.54	1.41	1.37
22	C	509	CLA	C1B-C2B	2.53	1.49	1.43
28	L	102	LHG	O7-C5	-2.53	1.40	1.46
22	c	508	CLA	C1D-ND	2.53	1.41	1.37
30	H	102	DGD	O1G-C1G	-2.53	1.39	1.45
24	C	514	BCR	C33-C5	-2.53	1.46	1.50
24	A	406	BCR	C33-C5	-2.53	1.46	1.50
22	C	504	CLA	C3B-C4B	2.53	1.50	1.42
22	b	607	CLA	C1B-C2B	2.52	1.49	1.43
28	d	406	LHG	O8-C6	-2.52	1.39	1.45
22	C	502	CLA	CMC-C2C	-2.51	1.45	1.50
22	b	609	CLA	CMD-C2D	-2.51	1.45	1.50
27	c	520	LMG	C1-C2	2.51	1.59	1.52
22	c	513	CLA	C1B-C2B	2.51	1.49	1.43
22	C	509	CLA	C1B-NB	-2.50	1.34	1.37
29	B	622	SQD	O2-C2	-2.50	1.36	1.43
30	h	101	DGD	O5D-C1E	2.50	1.44	1.40
22	C	502	CLA	C3B-C4B	2.50	1.50	1.42
30	C	516	DGD	O2D-C2D	-2.50	1.36	1.43
27	b	622	LMG	C1-C2	2.49	1.59	1.52
22	c	509	CLA	C1D-ND	2.49	1.41	1.37
27	c	520	LMG	O1-C1	2.49	1.44	1.40
22	b	611	CLA	CMD-C2D	-2.49	1.45	1.50
22	b	611	CLA	CMB-C2B	-2.49	1.45	1.50
22	A	402	CLA	CHC-C1C	2.49	1.43	1.38
22	B	601	CLA	CHC-C1C	2.48	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	409	LHG	O7-C5	-2.48	1.40	1.46
35	v	201	HEC	C3B-C2B	-2.48	1.32	1.41
28	E	101	LHG	C24-C23	2.48	1.57	1.50
24	k	103	BCR	C1-C6	-2.48	1.50	1.53
22	b	611	CLA	C1D-ND	2.48	1.41	1.37
26	d	405	PL9	C46-C44	-2.48	1.46	1.51
29	a	412	SQD	O2-C2	-2.47	1.36	1.43
22	C	503	CLA	CHC-C1C	2.47	1.43	1.38
22	a	405	CLA	C1B-NB	-2.47	1.34	1.37
22	c	505	CLA	CMD-C2D	-2.47	1.45	1.50
30	h	101	DGD	O5D-C6D	-2.47	1.39	1.43
22	C	512	CLA	C1B-C2B	2.47	1.48	1.43
29	a	412	SQD	O47-C7	2.47	1.41	1.34
22	C	510	CLA	C4B-NB	2.47	1.41	1.37
22	c	508	CLA	C4B-NB	2.47	1.41	1.37
22	B	615	CLA	C1B-C2B	2.46	1.48	1.43
28	d	407	LHG	P-O6	2.46	1.69	1.59
22	b	610	CLA	C1B-C2B	2.46	1.48	1.43
22	C	504	CLA	CMD-C2D	-2.46	1.45	1.50
22	B	611	CLA	CHC-C1C	2.46	1.43	1.38
22	d	403	CLA	MG-NB	-2.45	2.00	2.05
22	b	612	CLA	C1B-NB	-2.45	1.34	1.37
22	b	606	CLA	C1B-C2B	2.45	1.48	1.43
22	c	507	CLA	CMC-C2C	-2.45	1.45	1.50
22	b	603	CLA	CHC-C1C	2.45	1.43	1.38
30	H	102	DGD	O2D-C2D	-2.45	1.36	1.43
22	C	501	CLA	C1B-C2B	2.44	1.48	1.43
22	D	403	CLA	MG-NC	-2.44	2.00	2.06
22	a	402	CLA	CHC-C1C	2.44	1.43	1.38
22	b	607	CLA	C4B-NB	2.44	1.41	1.37
28	D	409	LHG	O8-C6	-2.44	1.39	1.45
22	d	402	CLA	C3B-C4B	2.43	1.49	1.42
22	C	506	CLA	CHC-C1C	2.43	1.43	1.38
22	c	512	CLA	CMC-C2C	-2.43	1.45	1.50
24	k	102	BCR	C33-C5	-2.42	1.47	1.50
22	b	610	CLA	C3D-C4D	2.42	1.49	1.44
22	A	403	CLA	MG-NB	-2.42	2.01	2.05
22	B	607	CLA	C3B-C4B	2.42	1.49	1.42
22	B	608	CLA	C4B-NB	2.42	1.41	1.37
22	b	605	CLA	C1B-C2B	2.42	1.48	1.43
22	c	506	CLA	CMD-C2D	-2.42	1.45	1.50
22	a	402	CLA	MG-NB	2.41	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	C4B-NB	2.41	1.41	1.37
22	a	411	CLA	CMA-C3A	-2.41	1.48	1.53
24	b	617	BCR	C33-C5	-2.41	1.47	1.50
22	c	513	CLA	CHC-C1C	2.41	1.43	1.38
22	C	508	CLA	MG-NB	2.40	2.10	2.05
22	B	606	CLA	C1B-C2B	2.40	1.48	1.43
22	b	610	CLA	MG-NC	2.40	2.12	2.06
30	h	101	DGD	O2D-C2D	-2.40	1.37	1.43
22	c	510	CLA	CAA-C2A	-2.40	1.49	1.54
22	c	512	CLA	CHC-C1C	2.40	1.43	1.38
27	m	101	LMG	O7-C8	-2.39	1.41	1.46
30	C	515	DGD	C3G-C2G	2.39	1.58	1.50
28	B	621	LHG	P-O6	2.39	1.68	1.59
30	c	517	DGD	O4D-C4D	-2.39	1.37	1.43
22	b	601	CLA	CHC-C1C	2.39	1.43	1.38
26	a	410	PL9	C40-C39	-2.39	1.44	1.50
22	b	610	CLA	MG-ND	-2.39	2.01	2.05
22	C	505	CLA	MG-ND	2.39	2.10	2.05
22	B	613	CLA	O2D-CED	-2.39	1.40	1.45
22	b	605	CLA	C1D-ND	2.39	1.41	1.37
22	c	501	CLA	CHC-C4B	-2.38	1.34	1.39
30	A	414	DGD	O2G-C1B	2.38	1.41	1.34
22	B	611	CLA	C3B-C4B	2.38	1.49	1.42
22	c	502	CLA	C1B-NB	-2.38	1.34	1.37
30	H	102	DGD	C6D-C5D	2.38	1.58	1.51
26	D	407	PL9	C3-C4	-2.38	1.45	1.49
22	b	607	CLA	CMC-C2C	-2.38	1.45	1.50
22	b	609	CLA	C1B-C2B	2.38	1.48	1.43
32	b	624	STE	O1-C1	2.38	1.29	1.22
22	c	503	CLA	CMB-C2B	-2.37	1.45	1.50
30	C	517	DGD	O2E-C2E	-2.37	1.37	1.43
30	C	515	DGD	C6D-C5D	2.37	1.58	1.51
22	b	602	CLA	CAC-C3C	-2.36	1.45	1.51
22	B	607	CLA	CMB-C2B	-2.36	1.45	1.50
22	C	505	CLA	C1D-ND	2.36	1.41	1.37
30	B	623	DGD	C2A-C1A	2.36	1.57	1.50
22	A	402	CLA	MG-ND	-2.36	2.01	2.05
34	e	101	HEM	CMA-C3A	2.36	1.55	1.50
22	C	501	CLA	C3B-C4B	2.36	1.49	1.42
34	F	101	HEM	CAB-C3B	2.36	1.53	1.47
22	a	402	CLA	C1D-C2D	2.35	1.50	1.45
22	c	501	CLA	CAC-C3C	-2.35	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	PHO	C3D-C4D	2.35	1.44	1.41
22	c	513	CLA	CMC-C2C	-2.35	1.45	1.50
30	C	517	DGD	O5D-C6D	2.35	1.47	1.43
22	a	403	CLA	CMD-C2D	-2.35	1.46	1.50
22	B	609	CLA	C4B-NB	2.35	1.40	1.37
22	B	605	CLA	C1B-NB	-2.35	1.34	1.37
24	T	101	BCR	C27-C26	-2.35	1.46	1.51
28	E	101	LHG	O7-C5	-2.35	1.41	1.46
30	H	102	DGD	O6D-C5D	-2.34	1.38	1.44
22	b	604	CLA	C1B-NB	-2.34	1.34	1.37
22	c	504	CLA	C1B-NB	-2.34	1.34	1.37
22	b	609	CLA	MG-NA	2.34	2.11	2.06
30	c	516	DGD	C6E-C5E	2.34	1.59	1.51
22	b	603	CLA	C4B-NB	2.34	1.40	1.37
22	B	609	CLA	O2D-CGD	2.33	1.39	1.33
22	b	611	CLA	MG-NB	-2.33	2.01	2.05
30	c	515	DGD	C6D-C5D	2.33	1.58	1.51
30	B	623	DGD	C3G-C2G	2.33	1.56	1.51
22	b	613	CLA	C1B-NB	-2.33	1.34	1.37
22	c	504	CLA	CHC-C1C	2.33	1.43	1.38
22	B	613	CLA	CMB-C2B	-2.32	1.46	1.50
22	c	501	CLA	C1D-ND	2.32	1.40	1.37
34	e	101	HEM	CAB-C3B	2.32	1.53	1.47
22	B	611	CLA	CMB-C2B	-2.32	1.46	1.50
22	b	607	CLA	C3B-C4B	2.32	1.49	1.42
22	B	609	CLA	CHD-C1D	-2.32	1.33	1.38
24	t	101	BCR	C27-C26	-2.32	1.46	1.51
22	c	510	CLA	CMC-C2C	-2.32	1.46	1.50
22	B	611	CLA	C1D-ND	2.32	1.40	1.37
22	A	403	CLA	C1B-NB	-2.32	1.34	1.37
24	b	618	BCR	C1-C6	-2.32	1.50	1.53
30	c	515	DGD	C3G-C2G	2.31	1.58	1.50
23	a	404	PHO	C3B-C2B	-2.31	1.37	1.40
22	B	612	CLA	MG-NB	-2.31	2.01	2.05
34	F	101	HEM	FE-NB	2.31	2.02	1.94
22	B	604	CLA	C1D-ND	2.31	1.40	1.37
22	B	601	CLA	CMB-C2B	-2.31	1.46	1.50
22	C	502	CLA	CMB-C2B	-2.31	1.46	1.50
30	C	515	DGD	O2D-C2D	-2.31	1.37	1.43
22	B	615	CLA	C1B-NB	-2.31	1.34	1.37
22	b	613	CLA	C1D-ND	2.31	1.40	1.37
22	B	609	CLA	CHC-C4B	-2.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	CAC-C3C	-2.31	1.47	1.51
22	b	614	CLA	CMC-C2C	-2.31	1.46	1.50
22	c	504	CLA	CMB-C2B	-2.31	1.46	1.50
22	b	603	CLA	MG-NB	-2.31	2.01	2.05
22	c	512	CLA	CMD-C2D	-2.31	1.46	1.50
22	D	404	CLA	CMD-C2D	-2.30	1.46	1.50
24	c	514	BCR	C33-C5	-2.30	1.47	1.50
30	H	102	DGD	O3G-C1D	2.30	1.44	1.40
22	b	610	CLA	CMC-C2C	-2.30	1.46	1.50
27	C	518	LMG	O7-C8	-2.30	1.41	1.46
29	F	102	SQD	O3-C3	-2.30	1.37	1.43
22	b	603	CLA	CMC-C2C	-2.30	1.46	1.50
22	b	607	CLA	CMD-C2D	-2.30	1.46	1.50
22	d	402	CLA	CHC-C1C	2.29	1.43	1.38
22	b	613	CLA	CHC-C4B	-2.29	1.34	1.39
22	B	616	CLA	C1B-C2B	2.29	1.48	1.43
27	D	408	LMG	C4-C3	2.29	1.58	1.52
27	D	408	LMG	C1-C2	2.29	1.59	1.52
22	d	403	CLA	CMC-C2C	-2.29	1.46	1.50
22	a	411	CLA	C1B-C2B	2.29	1.48	1.43
22	b	614	CLA	C1B-C2B	2.29	1.48	1.43
34	e	101	HEM	CAC-C3C	2.29	1.53	1.47
23	A	404	PHO	O2D-CGD	2.29	1.38	1.33
22	C	508	CLA	CMD-C2D	-2.29	1.46	1.50
22	C	501	CLA	CHC-C1C	2.28	1.43	1.38
29	F	102	SQD	O2-C2	-2.28	1.37	1.43
26	D	407	PL9	C32-C33	-2.28	1.43	1.50
22	C	503	CLA	C3B-C4B	2.28	1.49	1.42
22	b	615	CLA	C1B-C2B	2.28	1.48	1.43
24	B	618	BCR	C33-C5	-2.27	1.47	1.50
22	B	602	CLA	CMB-C2B	-2.27	1.46	1.50
22	B	610	CLA	CHC-C1C	2.27	1.43	1.38
22	c	509	CLA	CMB-C2B	-2.27	1.46	1.50
22	b	612	CLA	MG-NB	-2.27	2.01	2.05
22	b	602	CLA	C3B-C4B	2.27	1.49	1.42
32	B	620	STE	C2-C1	2.27	1.55	1.50
22	b	601	CLA	O2A-CGA	2.27	1.40	1.33
22	B	605	CLA	CMC-C2C	-2.26	1.46	1.50
24	b	618	BCR	C33-C5	-2.26	1.47	1.50
22	b	608	CLA	C1D-C2D	2.26	1.49	1.45
26	d	405	PL9	C7-C3	2.26	1.54	1.51
22	c	508	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	C3B-C4B	2.26	1.49	1.42
22	C	503	CLA	C4B-NB	2.26	1.40	1.37
22	c	511	CLA	CMB-C2B	-2.26	1.46	1.50
27	C	518	LMG	C3-C2	2.26	1.58	1.52
22	a	405	CLA	C3B-C4B	2.26	1.49	1.42
22	C	504	CLA	CHC-C4B	-2.26	1.34	1.39
26	D	407	PL9	C35-C34	-2.26	1.45	1.50
22	C	510	CLA	C1B-C2B	2.26	1.48	1.43
27	a	414	LMG	O7-C8	-2.26	1.41	1.46
23	D	401	PHO	CMC-C2C	-2.26	1.47	1.50
30	C	515	DGD	O1G-C1A	2.25	1.39	1.33
22	b	609	CLA	C3B-C4B	2.25	1.49	1.42
22	A	405	CLA	MG-ND	2.25	2.10	2.05
22	A	403	CLA	C3B-C4B	2.25	1.49	1.42
30	c	515	DGD	O6E-C1E	-2.25	1.36	1.41
30	c	517	DGD	C4E-C3E	-2.25	1.46	1.52
22	b	614	CLA	CMB-C2B	-2.25	1.46	1.50
23	A	404	PHO	CAC-C3C	-2.25	1.47	1.51
22	b	616	CLA	C1B-NB	-2.24	1.34	1.37
22	b	603	CLA	C1B-C2B	2.24	1.48	1.43
22	B	601	CLA	CMC-C2C	-2.24	1.46	1.50
23	D	401	PHO	C4D-CHA	2.24	1.42	1.39
22	c	513	CLA	CMB-C2B	-2.24	1.46	1.50
22	c	509	CLA	C1B-NB	-2.24	1.34	1.37
22	C	507	CLA	CMC-C2C	-2.23	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.23	1.46	1.50
24	Z	101	BCR	C33-C5	-2.23	1.47	1.50
28	e	102	LHG	C6-C5	2.23	1.57	1.50
22	b	606	CLA	CMB-C2B	-2.23	1.46	1.50
23	d	401	PHO	C4D-CHA	2.23	1.42	1.39
24	T	101	BCR	C1-C6	-2.23	1.50	1.53
22	C	502	CLA	MG-NB	-2.23	2.01	2.05
22	b	607	CLA	O2D-CED	-2.22	1.40	1.45
22	b	608	CLA	CMA-C3A	-2.22	1.48	1.53
30	C	516	DGD	O5D-C6D	-2.22	1.39	1.43
30	H	102	DGD	C3E-C2E	2.22	1.58	1.52
22	C	502	CLA	C4B-NB	2.22	1.40	1.37
26	D	407	PL9	C26-C24	-2.22	1.46	1.51
22	c	502	CLA	MG-NC	-2.22	2.01	2.06
22	c	502	CLA	C4B-NB	2.22	1.40	1.37
24	T	101	BCR	C38-C26	-2.21	1.47	1.50
22	C	507	CLA	CMB-C2B	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	MG-NB	-2.21	2.01	2.05
30	h	101	DGD	C1E-C2E	2.21	1.59	1.52
22	c	513	CLA	MG-NA	-2.21	2.01	2.06
30	A	414	DGD	O1G-C1G	-2.21	1.40	1.45
23	D	401	PHO	C1D-ND	2.20	1.42	1.38
22	c	502	CLA	CMC-C2C	-2.20	1.46	1.50
23	a	404	PHO	CMC-C2C	-2.20	1.47	1.50
24	a	406	BCR	C33-C5	-2.20	1.47	1.50
34	e	101	HEM	C2A-C3A	-2.20	1.33	1.38
22	A	402	CLA	CMC-C2C	-2.20	1.46	1.50
30	C	515	DGD	C2A-C1A	-2.20	1.44	1.50
22	B	613	CLA	MG-NC	2.20	2.11	2.06
22	c	510	CLA	CMD-C2D	-2.20	1.46	1.50
22	C	506	CLA	C3B-C4B	2.20	1.49	1.42
22	b	615	CLA	CHC-C4B	-2.19	1.34	1.39
22	b	616	CLA	C3D-C4D	2.19	1.49	1.44
22	c	511	CLA	C3B-C4B	2.19	1.49	1.42
30	c	517	DGD	C6D-C5D	2.19	1.58	1.51
22	c	508	CLA	C1B-C2B	2.19	1.48	1.43
24	B	617	BCR	C33-C5	-2.19	1.47	1.50
22	B	611	CLA	C4B-NB	2.19	1.40	1.37
22	C	508	CLA	C3B-C4B	2.19	1.49	1.42
24	b	618	BCR	C36-C18	-2.19	1.46	1.50
24	H	101	BCR	C1-C6	-2.19	1.51	1.53
23	a	404	PHO	C4D-CHA	2.19	1.42	1.39
22	D	403	CLA	C1D-ND	2.19	1.40	1.37
34	F	101	HEM	CMD-C2D	2.19	1.55	1.50
28	b	623	LHG	C24-C23	2.19	1.57	1.50
22	c	507	CLA	CMB-C2B	-2.19	1.46	1.50
22	c	501	CLA	CMD-C2D	-2.19	1.46	1.50
24	C	514	BCR	C36-C18	-2.18	1.46	1.50
22	B	613	CLA	C1B-C2B	2.18	1.48	1.43
22	b	605	CLA	CMD-C2D	-2.18	1.46	1.50
22	c	504	CLA	CMD-C2D	-2.18	1.46	1.50
22	C	503	CLA	CMB-C2B	-2.18	1.46	1.50
22	C	503	CLA	CMD-C2D	-2.18	1.46	1.50
23	a	404	PHO	O2D-CGD	2.18	1.38	1.33
22	b	607	CLA	CHC-C1C	2.17	1.42	1.38
27	d	408	LMG	O7-C10	2.17	1.38	1.30
22	B	612	CLA	C3B-C4B	2.17	1.49	1.42
27	d	409	LMG	O8-C28	2.17	1.39	1.33
22	c	507	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	O2D-CGD	2.17	1.38	1.33
27	C	518	LMG	O1-C1	2.17	1.43	1.40
22	b	606	CLA	CHC-C4B	-2.17	1.34	1.39
22	C	513	CLA	CMD-C2D	-2.17	1.46	1.50
28	e	102	LHG	O8-C23	2.17	1.39	1.33
22	B	602	CLA	OBD-CAD	2.17	1.26	1.22
22	B	608	CLA	CMD-C2D	-2.16	1.46	1.50
27	c	520	LMG	O6-C1	2.16	1.47	1.41
26	d	405	PL9	C11-C9	-2.16	1.46	1.51
22	B	616	CLA	MG-NC	2.16	2.11	2.06
22	b	613	CLA	O2D-CED	-2.16	1.40	1.45
22	a	411	CLA	C3B-C4B	2.16	1.49	1.42
24	K	102	BCR	C38-C26	-2.16	1.47	1.50
22	b	608	CLA	C3B-C4B	2.16	1.49	1.42
23	a	404	PHO	C3D-C4D	2.15	1.44	1.41
22	C	510	CLA	C3D-C4D	2.15	1.49	1.44
23	a	404	PHO	CMD-C2D	-2.15	1.47	1.51
22	c	509	CLA	CMD-C2D	-2.15	1.46	1.50
35	v	201	HEC	CMB-C2B	2.15	1.55	1.50
22	B	603	CLA	C1B-NB	-2.15	1.35	1.37
24	B	619	BCR	C33-C5	-2.15	1.47	1.50
22	B	607	CLA	C1B-C2B	2.15	1.48	1.43
22	c	510	CLA	C1B-C2B	2.15	1.48	1.43
22	D	405	CLA	C4B-NB	2.15	1.40	1.37
22	D	403	CLA	O2D-CED	-2.15	1.40	1.45
23	D	401	PHO	CAC-C3C	-2.14	1.48	1.51
22	C	512	CLA	C4B-NB	2.14	1.40	1.37
22	B	602	CLA	C3B-C4B	2.14	1.49	1.42
29	f	101	SQD	O2-C2	-2.14	1.37	1.43
22	B	614	CLA	C1A-CHA	-2.14	1.34	1.43
28	d	407	LHG	O6-C4	-2.14	1.36	1.44
22	c	503	CLA	CHC-C1C	2.14	1.42	1.38
22	B	608	CLA	C1B-C2B	2.14	1.48	1.43
22	b	614	CLA	C3B-C4B	2.14	1.49	1.42
22	B	605	CLA	MG-NA	2.14	2.11	2.06
22	c	511	CLA	C3D-C4D	2.14	1.49	1.44
22	C	504	CLA	O2D-CGD	2.14	1.38	1.33
35	v	201	HEC	C3C-C2C	-2.14	1.34	1.41
22	c	513	CLA	MG-NC	2.14	2.11	2.06
22	a	411	CLA	CMB-C2B	-2.13	1.46	1.50
22	c	502	CLA	C1B-C2B	2.13	1.48	1.43
22	a	405	CLA	CHC-C4B	-2.13	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	MG-NC	-2.13	2.01	2.06
22	C	513	CLA	CHC-C1C	2.13	1.42	1.38
22	d	403	CLA	C1B-C2B	2.13	1.48	1.43
22	C	510	CLA	MG-NB	-2.13	2.01	2.05
30	h	101	DGD	C4D-C3D	2.13	1.57	1.52
30	C	516	DGD	O2G-C2G	-2.13	1.41	1.46
22	C	510	CLA	CMD-C2D	-2.13	1.46	1.50
22	d	403	CLA	CHC-C4B	-2.13	1.34	1.39
24	T	101	BCR	C4-C5	-2.13	1.47	1.51
22	b	609	CLA	CMC-C2C	-2.13	1.46	1.50
22	B	607	CLA	C1C-NC	-2.12	1.34	1.37
32	a	415	STE	O1-C1	2.12	1.29	1.22
30	H	102	DGD	C4D-C3D	2.12	1.57	1.52
22	b	616	CLA	O2D-CED	-2.12	1.40	1.45
22	d	403	CLA	CHC-C1C	2.12	1.42	1.38
22	B	602	CLA	C1B-C2B	2.12	1.48	1.43
23	D	401	PHO	O2D-CGD	2.12	1.38	1.33
22	B	613	CLA	C3B-C4B	2.12	1.48	1.42
22	b	604	CLA	C1D-ND	2.12	1.40	1.37
35	V	201	HEC	C3B-C2B	-2.12	1.34	1.41
22	C	505	CLA	CMC-C2C	-2.11	1.46	1.50
30	C	516	DGD	O4D-C4D	-2.11	1.37	1.43
27	C	518	LMG	O8-C9	-2.11	1.40	1.45
23	d	401	PHO	CMB-C2B	-2.11	1.47	1.51
24	Z	101	BCR	C4-C5	-2.11	1.47	1.51
22	B	608	CLA	CMC-C2C	-2.11	1.46	1.50
23	d	401	PHO	CAA-C2A	-2.11	1.49	1.54
22	C	513	CLA	C3B-C4B	2.11	1.48	1.42
22	c	506	CLA	C1B-NB	-2.11	1.35	1.37
22	C	509	CLA	O2D-CGD	2.11	1.38	1.33
22	c	508	CLA	CMA-C3A	-2.10	1.48	1.53
22	A	405	CLA	CAC-C3C	-2.10	1.45	1.51
35	v	201	HEC	CMD-C2D	2.10	1.55	1.50
30	c	515	DGD	C3E-C2E	2.10	1.57	1.52
22	B	613	CLA	CAB-C3B	-2.10	1.41	1.47
22	b	615	CLA	C1D-ND	2.10	1.40	1.37
28	D	409	LHG	P-O3	2.10	1.67	1.59
30	h	101	DGD	O2E-C2E	-2.10	1.37	1.43
22	C	510	CLA	CMB-C2B	-2.10	1.46	1.50
27	b	622	LMG	C9-C8	2.10	1.57	1.50
22	B	604	CLA	C4C-C3C	2.10	1.48	1.45
22	c	506	CLA	CAA-C2A	-2.10	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	405	CLA	CMC-C2C	-2.09	1.46	1.50
30	C	517	DGD	C6D-C5D	2.09	1.57	1.51
22	C	510	CLA	O2A-CGA	2.09	1.39	1.33
22	C	511	CLA	CHC-C1C	2.09	1.42	1.38
23	D	401	PHO	CAA-C2A	-2.09	1.49	1.54
23	A	404	PHO	CHA-CBD	-2.09	1.49	1.51
22	b	613	CLA	C1B-C2B	2.08	1.48	1.43
22	b	604	CLA	C3B-C4B	2.08	1.48	1.42
22	c	506	CLA	CHC-C4B	-2.08	1.34	1.39
22	C	505	CLA	C3B-C4B	2.08	1.48	1.42
22	C	505	CLA	O2D-CED	-2.08	1.40	1.45
22	c	501	CLA	C4B-NB	2.08	1.40	1.37
22	C	513	CLA	C1D-C2D	2.08	1.49	1.45
22	A	403	CLA	MG-ND	-2.08	2.01	2.05
24	B	617	BCR	C38-C26	-2.08	1.47	1.50
22	D	404	CLA	CMB-C2B	-2.08	1.46	1.50
30	A	414	DGD	C1E-C2E	2.07	1.58	1.52
24	c	514	BCR	C38-C26	-2.07	1.47	1.50
26	D	407	PL9	C41-C39	-2.07	1.47	1.51
22	C	513	CLA	CHC-C4B	-2.07	1.34	1.39
34	F	101	HEM	CMB-C2B	2.07	1.55	1.50
22	b	615	CLA	C4-C3	-2.07	1.45	1.50
22	C	510	CLA	C3B-C4B	2.07	1.48	1.42
22	b	603	CLA	O2D-CGD	2.07	1.38	1.33
22	B	613	CLA	CHC-C1C	2.07	1.42	1.38
22	c	504	CLA	CMC-C2C	-2.07	1.46	1.50
22	C	509	CLA	C3B-C4B	2.07	1.48	1.42
22	B	605	CLA	C3B-C4B	2.06	1.48	1.42
29	A	412	SQD	O3-C3	-2.06	1.37	1.43
29	f	101	SQD	O3-C3	-2.06	1.37	1.43
22	B	605	CLA	O2D-CED	-2.06	1.40	1.45
22	C	506	CLA	CMD-C2D	-2.06	1.46	1.50
32	k	104	STE	C2-C1	2.06	1.55	1.50
22	B	606	CLA	CMA-C3A	-2.06	1.48	1.53
30	c	515	DGD	O1G-C1A	2.05	1.39	1.33
22	D	405	CLA	C3B-C4B	2.05	1.48	1.42
22	b	603	CLA	C1A-CHA	-2.05	1.34	1.43
28	E	101	LHG	O8-C6	-2.05	1.40	1.45
22	B	603	CLA	C3B-C4B	2.05	1.48	1.42
27	c	518	LMG	O8-C9	-2.05	1.40	1.45
22	b	610	CLA	CHC-C4B	-2.05	1.34	1.39
23	A	404	PHO	CMA-C3A	-2.05	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	CMB-C2B	-2.05	1.46	1.50
22	a	403	CLA	C1B-C2B	2.05	1.47	1.43
22	b	616	CLA	CMC-C2C	-2.04	1.46	1.50
27	b	622	LMG	C4-C5	2.04	1.57	1.53
22	B	609	CLA	C3B-C4B	2.04	1.48	1.42
22	c	508	CLA	CHC-C1C	2.04	1.42	1.38
24	A	406	BCR	C38-C26	-2.04	1.47	1.50
22	b	608	CLA	CHC-C1C	2.04	1.42	1.38
22	b	614	CLA	O2D-CED	-2.04	1.40	1.45
22	C	507	CLA	CHC-C1C	2.04	1.42	1.38
22	c	508	CLA	C1B-NB	-2.04	1.35	1.37
22	c	501	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	602	CLA	MG-NA	-2.04	2.01	2.06
22	B	605	CLA	CHC-C4B	-2.04	1.34	1.39
22	b	606	CLA	O2D-CED	-2.04	1.40	1.45
22	a	403	CLA	O2D-CED	-2.04	1.40	1.45
30	c	517	DGD	C3E-C2E	2.04	1.57	1.52
28	A	411	LHG	O8-C23	2.04	1.39	1.33
22	D	405	CLA	CMD-C2D	-2.04	1.46	1.50
24	b	618	BCR	C27-C26	-2.04	1.47	1.51
22	b	615	CLA	CHC-C1C	2.04	1.42	1.38
22	C	502	CLA	CAC-C3C	-2.03	1.45	1.51
22	b	613	CLA	C3B-C4B	2.03	1.48	1.42
22	c	505	CLA	CMC-C2C	-2.03	1.46	1.50
22	C	513	CLA	C4B-NB	2.03	1.40	1.37
22	b	607	CLA	C1B-NB	-2.03	1.35	1.37
22	C	504	CLA	CHC-C1C	2.03	1.42	1.38
22	C	509	CLA	O2A-CGA	2.03	1.39	1.33
22	c	502	CLA	CHC-C1C	2.03	1.42	1.38
23	d	401	PHO	CBD-CGD	-2.03	1.49	1.52
22	B	616	CLA	CHC-C4B	-2.03	1.34	1.39
22	C	506	CLA	C1B-NB	-2.02	1.35	1.37
22	B	607	CLA	CMC-C2C	-2.02	1.46	1.50
22	C	512	CLA	C3B-C4B	2.02	1.48	1.42
29	A	412	SQD	O4-C4	-2.02	1.38	1.43
22	A	403	CLA	CMB-C2B	-2.02	1.46	1.50
22	C	507	CLA	C1B-NB	-2.02	1.35	1.37
22	c	508	CLA	O2D-CGD	2.01	1.38	1.33
22	c	507	CLA	C1D-ND	2.01	1.40	1.37
22	c	505	CLA	CHC-C1C	2.01	1.42	1.38
32	b	625	STE	O1-C1	2.01	1.28	1.22
28	b	623	LHG	O8-C23	2.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	C4B-NB	2.01	1.40	1.37
22	B	605	CLA	C1C-NC	-2.01	1.34	1.37
22	c	502	CLA	C1D-ND	2.01	1.40	1.37
27	b	622	LMG	C7-C8	2.01	1.57	1.50
24	C	514	BCR	C38-C26	-2.01	1.47	1.50
22	c	508	CLA	CMB-C2B	-2.01	1.46	1.50
22	b	605	CLA	CHC-C4B	-2.01	1.34	1.39
30	h	101	DGD	O1G-C1G	-2.01	1.40	1.45
30	c	516	DGD	C3G-C2G	2.01	1.57	1.50
27	A	410	LMG	C4-C5	2.01	1.57	1.53
22	a	411	CLA	MG-NB	2.00	2.09	2.05
22	B	601	CLA	C1D-C2D	2.00	1.49	1.45
28	B	621	LHG	O8-C6	-2.00	1.40	1.45
22	C	513	CLA	CMC-C2C	-2.00	1.46	1.50
27	a	414	LMG	O8-C9	-2.00	1.40	1.45
27	A	410	LMG	O6-C5	-2.00	1.39	1.44
22	c	506	CLA	CMB-C2B	-2.00	1.46	1.50

All (1221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	V	201	HEC	CBB-CAB-C3B	-11.03	105.38	127.43
22	C	503	CLA	C4A-NA-C1A	10.19	111.33	106.68
22	B	616	CLA	C4A-NA-C1A	9.47	111.00	106.68
29	a	412	SQD	O6-C1-C2	8.95	121.87	108.27
29	A	412	SQD	O6-C1-C2	8.85	121.72	108.27
22	B	606	CLA	C4A-NA-C1A	8.78	110.69	106.68
35	v	201	HEC	CBB-CAB-C3B	-8.70	110.05	127.43
29	L	101	SQD	O6-C1-C2	8.67	121.44	108.27
22	B	604	CLA	C4A-NA-C1A	8.18	110.41	106.68
22	b	604	CLA	C4A-NA-C1A	7.89	110.28	106.68
35	v	201	HEC	CBC-CAC-C3C	-7.81	111.82	127.43
22	D	403	CLA	C4A-NA-C1A	7.73	110.21	106.68
22	b	606	CLA	C4A-NA-C1A	7.70	110.19	106.68
22	b	616	CLA	C4A-NA-C1A	7.66	110.17	106.68
22	d	402	CLA	C4A-NA-C1A	7.63	110.16	106.68
35	V	201	HEC	CBC-CAC-C3C	-7.58	112.28	127.43
22	c	503	CLA	C4A-NA-C1A	7.46	110.08	106.68
29	B	622	SQD	O6-C1-C2	7.35	119.43	108.27
22	C	509	CLA	C4A-NA-C1A	7.17	109.95	106.68
22	b	601	CLA	C4A-NA-C1A	7.14	109.94	106.68
22	B	607	CLA	C4A-NA-C1A	7.07	109.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	PL9	C7-C3-C4	6.95	122.63	116.91
22	b	609	CLA	C4A-NA-C1A	6.94	109.85	106.68
22	c	501	CLA	C4A-NA-C1A	6.77	109.77	106.68
26	d	405	PL9	C7-C3-C4	6.64	122.38	116.91
22	C	507	CLA	C4A-NA-C1A	6.59	109.69	106.68
22	c	508	CLA	C4A-NA-C1A	6.51	109.65	106.68
22	c	510	CLA	C4A-NA-C1A	6.49	109.64	106.68
22	c	511	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	b	607	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	B	601	CLA	C4A-NA-C1A	6.37	109.58	106.68
29	F	102	SQD	O6-C1-C2	6.31	117.86	108.27
22	C	502	CLA	C4A-NA-C1A	6.25	109.53	106.68
26	D	407	PL9	C7-C3-C4	6.20	122.02	116.91
22	c	507	CLA	C4A-NA-C1A	6.18	109.50	106.68
22	C	511	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	C	510	CLA	C4A-NA-C1A	6.03	109.43	106.68
22	b	614	CLA	C4A-NA-C1A	5.94	109.39	106.68
22	B	615	CLA	C4A-NA-C1A	5.85	109.35	106.68
22	B	609	CLA	C4A-NA-C1A	5.85	109.35	106.68
22	a	403	CLA	C4A-NA-C1A	5.83	109.34	106.68
22	C	512	CLA	C4A-NA-C1A	5.76	109.31	106.68
22	b	605	CLA	C4A-NA-C1A	5.69	109.28	106.68
29	f	101	SQD	O7-S-C6	5.63	115.16	106.76
22	b	602	CLA	C4A-NA-C1A	5.58	109.22	106.68
22	c	509	CLA	C4A-NA-C1A	5.54	109.21	106.68
22	D	404	CLA	C4A-NA-C1A	5.51	109.19	106.68
22	B	611	CLA	C4A-NA-C1A	5.43	109.16	106.68
22	B	605	CLA	C4A-NA-C1A	5.36	109.12	106.68
22	c	503	CLA	C3B-C4B-NB	-5.28	105.81	110.53
23	A	404	PHO	C4D-CHA-CBD	-5.28	105.92	108.45
22	b	615	CLA	C4A-NA-C1A	5.24	109.07	106.68
29	L	101	SQD	O7-S-C6	5.23	114.56	106.76
29	f	101	SQD	O6-C1-C2	5.21	116.19	108.27
29	B	622	SQD	O47-C7-C8	5.20	122.73	111.48
22	b	602	CLA	O2D-CGD-O1D	-5.18	113.77	123.85
22	b	606	CLA	O2D-CGD-O1D	-5.18	113.77	123.85
22	B	612	CLA	C4A-NA-C1A	5.18	109.04	106.68
29	A	413	SQD	C45-O47-C7	5.08	125.10	117.78
26	A	409	PL9	C40-C39-C41	5.06	124.02	115.23
22	A	405	CLA	C4A-NA-C1A	5.05	108.98	106.68
22	b	611	CLA	C4A-NA-C1A	5.05	108.98	106.68
22	B	603	CLA	C4A-NA-C1A	5.00	108.96	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	405	CLA	C4A-NA-C1A	4.98	108.95	106.68
22	c	505	CLA	C4A-NA-C1A	4.97	108.95	106.68
22	B	614	CLA	O2D-CGD-O1D	-4.97	114.18	123.85
23	a	404	PHO	C4D-CHA-CBD	-4.92	106.09	108.45
22	b	610	CLA	C4A-NA-C1A	4.90	108.91	106.68
22	C	505	CLA	C4A-NA-C1A	4.89	108.91	106.68
26	a	410	PL9	C7-C3-C2	-4.89	117.63	123.39
29	A	412	SQD	O7-S-C6	4.84	113.99	106.76
22	C	513	CLA	O2D-CGD-O1D	-4.80	114.50	123.85
22	c	512	CLA	C1-C2-C3	-4.80	118.33	126.20
22	a	405	CLA	C4A-NA-C1A	4.75	108.85	106.68
29	a	413	SQD	O47-C7-C8	4.59	121.42	111.48
29	F	102	SQD	O9-S-C6	4.59	113.60	106.76
22	a	411	CLA	C4A-NA-C1A	4.57	108.76	106.68
28	D	409	LHG	O4-P-O5	4.54	133.57	112.44
22	b	609	CLA	CMB-C2B-C1B	-4.54	118.51	125.42
30	c	517	DGD	O5D-C1E-C2E	4.53	115.15	108.27
22	b	611	CLA	O2D-CGD-O1D	-4.53	115.03	123.85
28	L	102	LHG	O4-P-O5	4.52	133.45	112.44
28	l	101	LHG	O4-P-O5	4.50	133.39	112.44
22	b	604	CLA	C1-C2-C3	-4.48	118.86	126.20
24	b	617	BCR	C2-C1-C6	4.46	116.91	110.44
22	A	402	CLA	CHB-C4A-NA	4.45	130.82	124.40
28	d	407	LHG	O4-P-O5	4.45	133.13	112.44
23	A	404	PHO	C2B-C1B-NB	-4.44	106.22	109.43
22	b	601	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
26	d	405	PL9	C40-C39-C41	4.41	122.88	115.23
22	b	603	CLA	O2D-CGD-O1D	-4.40	115.28	123.85
28	B	621	LHG	O4-P-O5	4.39	132.85	112.44
33	a	409	BCT	O2-C-O1	4.38	130.88	119.68
30	H	102	DGD	O3G-C3G-C2G	-4.37	100.18	110.82
30	C	515	DGD	O3G-C3G-C2G	-4.35	100.23	110.82
28	e	102	LHG	O4-P-O5	4.31	132.50	112.44
28	d	406	LHG	O4-P-O5	4.30	132.45	112.44
22	D	405	CLA	O2D-CGD-O1D	-4.30	115.48	123.85
22	b	611	CLA	O2D-CGD-CBD	4.26	118.67	111.23
29	L	101	SQD	O9-S-C6	4.25	113.09	106.76
29	F	102	SQD	C1-C2-C3	-4.23	101.12	110.01
27	b	622	LMG	C1-O6-C5	-4.22	105.47	113.72
22	b	603	CLA	C3B-C4B-NB	-4.21	106.77	110.53
29	A	412	SQD	O47-C7-C8	4.19	120.55	111.48
22	B	610	CLA	C4A-NA-C1A	4.18	108.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	O2A-CGA-O1A	-4.17	113.19	123.63
22	c	513	CLA	C4A-NA-C1A	4.16	108.58	106.68
29	a	412	SQD	O7-S-C6	4.16	112.97	106.76
22	A	405	CLA	O2D-CGD-CBD	4.15	118.48	111.23
22	C	506	CLA	C4A-NA-C1A	4.14	108.57	106.68
22	b	613	CLA	C1-C2-C3	-4.14	119.42	126.20
23	d	401	PHO	C4D-CHA-CBD	-4.11	106.48	108.45
28	E	101	LHG	O4-P-O5	4.11	131.54	112.44
22	B	613	CLA	C4A-NA-C1A	4.10	108.55	106.68
22	a	402	CLA	C4A-NA-C1A	4.10	108.55	106.68
26	D	407	PL9	C7-C3-C2	-4.08	118.58	123.39
28	A	411	LHG	O4-P-O5	4.08	131.42	112.44
22	c	501	CLA	O2D-CGD-O1D	-4.08	115.92	123.85
23	a	404	PHO	C2B-C1B-NB	-4.07	106.49	109.43
22	b	603	CLA	C4A-NA-C1A	4.06	108.53	106.68
22	c	512	CLA	C4A-NA-C1A	4.05	108.53	106.68
22	C	512	CLA	C3B-C4B-NB	-4.05	106.92	110.53
22	c	506	CLA	C4A-NA-C1A	4.04	108.52	106.68
29	A	412	SQD	C1-C2-C3	-4.04	101.52	110.01
34	F	101	HEM	CBD-CAD-C3D	-4.00	101.48	112.53
24	k	101	BCR	C2-C1-C6	3.99	116.23	110.44
29	L	101	SQD	O47-C7-C8	3.99	120.11	111.48
22	B	614	CLA	C3B-C4B-NB	-3.98	106.97	110.53
22	b	614	CLA	C3B-C4B-NB	-3.95	107.00	110.53
22	b	615	CLA	C3B-C4B-NB	-3.95	107.01	110.53
22	b	601	CLA	CHB-C4A-NA	3.92	130.06	124.40
22	D	404	CLA	C3B-C4B-NB	-3.92	107.03	110.53
22	c	504	CLA	C4A-NA-C1A	3.91	108.46	106.68
29	f	101	SQD	O9-S-O7	-3.90	101.15	113.82
22	C	503	CLA	C3B-C4B-NB	-3.88	107.07	110.53
22	B	601	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
22	C	508	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
28	b	623	LHG	O4-P-O5	3.85	130.37	112.44
22	c	512	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
22	B	608	CLA	C4A-NA-C1A	3.84	108.43	106.68
24	B	619	BCR	C2-C1-C6	3.82	116.00	110.44
27	m	101	LMG	O3-C3-C2	-3.82	101.36	110.38
34	e	101	HEM	CBA-CAA-C2A	-3.82	101.98	112.53
23	D	401	PHO	O1D-CGD-CBD	3.81	130.50	124.72
22	a	403	CLA	C3B-C4B-NB	-3.80	107.14	110.53
22	C	510	CLA	C3B-C4B-NB	-3.77	107.17	110.53
22	a	411	CLA	C3B-C4B-NB	-3.77	107.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	CMB-C2B-C1B	-3.76	119.69	125.42
26	A	409	PL9	C22-C23-C24	-3.76	119.02	127.62
22	B	606	CLA	C3B-C4B-NB	-3.75	107.18	110.53
22	c	512	CLA	CHB-C4A-NA	3.74	129.79	124.40
22	c	510	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
22	B	605	CLA	O1D-CGD-CBD	3.73	131.88	124.52
30	c	517	DGD	O3G-C3G-C2G	-3.73	101.76	110.82
22	c	505	CLA	C3B-C4B-NB	-3.72	107.20	110.53
23	A	404	PHO	OBD-CAD-C3D	3.72	133.70	127.89
30	C	516	DGD	O3G-C3G-C2G	-3.70	101.81	110.82
24	Z	101	BCR	C15-C16-C17	-3.70	115.95	123.52
29	B	622	SQD	C1-O5-C5	-3.70	106.49	113.72
29	A	412	SQD	O8-S-C6	3.70	113.11	105.97
22	B	613	CLA	C1-C2-C3	-3.68	120.17	126.20
22	C	512	CLA	CHB-C4A-NA	3.68	129.71	124.40
22	a	411	CLA	CHB-C4A-NA	3.68	129.71	124.40
33	D	402	BCT	O2-C-O1	3.68	129.08	119.68
22	B	602	CLA	CHB-C4A-NA	3.67	129.70	124.40
22	b	601	CLA	O2D-CGD-CBD	3.66	117.63	111.23
22	B	614	CLA	C4A-NA-C1A	3.65	108.34	106.68
22	c	505	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
22	C	511	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
22	C	505	CLA	CAC-C3C-C4C	3.63	129.51	124.79
22	b	613	CLA	C4A-NA-C1A	3.61	108.33	106.68
24	b	617	BCR	C38-C26-C25	-3.61	120.54	124.48
29	B	622	SQD	O9-S-O7	-3.60	102.10	113.82
22	A	405	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
27	C	518	LMG	O6-C1-O1	-3.60	101.55	110.04
22	b	616	CLA	CHB-C4A-NA	3.59	129.59	124.40
29	A	413	SQD	O48-C23-C24	3.58	122.76	111.83
23	D	401	PHO	C4D-CHA-CBD	-3.58	106.74	108.45
30	C	516	DGD	O2D-C2D-C1D	-3.57	101.56	110.08
30	h	101	DGD	O6E-C5E-C4E	3.57	116.14	109.70
22	b	613	CLA	CHB-C4A-NA	3.56	129.54	124.40
22	a	411	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
22	B	616	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
24	H	101	BCR	C38-C26-C25	-3.55	120.61	124.48
29	F	102	SQD	O8-S-C6	3.54	112.81	105.97
28	e	102	LHG	O8-C23-C24	3.53	122.61	111.83
24	H	101	BCR	C2-C1-C6	3.53	115.57	110.44
22	b	616	CLA	C3B-C4B-NB	-3.53	107.38	110.53
23	d	401	PHO	CMB-C2B-C3B	3.53	131.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	BCR	C29-C30-C25	3.52	115.55	110.44
23	d	401	PHO	C2B-C1B-NB	-3.52	106.89	109.43
30	A	414	DGD	O3G-C3G-C2G	-3.51	102.27	110.82
30	C	517	DGD	O3G-C3G-C2G	-3.51	102.27	110.82
22	C	504	CLA	C4A-NA-C1A	3.49	108.27	106.68
22	b	603	CLA	O2D-CGD-CBD	3.48	117.32	111.23
24	C	514	BCR	C2-C1-C6	3.48	115.49	110.44
22	D	405	CLA	CMB-C2B-C1B	-3.48	120.12	125.42
22	B	610	CLA	C3B-C4B-NB	-3.48	107.42	110.53
23	d	401	PHO	O1D-CGD-CBD	3.47	129.99	124.72
29	B	622	SQD	O7-S-C6	3.46	111.92	106.76
29	L	101	SQD	C1-C2-C3	-3.46	102.73	110.01
22	b	612	CLA	CMB-C2B-C1B	-3.46	120.15	125.42
22	C	508	CLA	C4A-NA-C1A	3.46	108.26	106.68
22	C	503	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
27	m	101	LMG	O1-C1-C2	-3.45	103.03	108.27
22	a	411	CLA	C1D-ND-C4D	3.45	108.73	106.31
22	A	402	CLA	C7-C6-C5	-3.45	104.07	113.26
22	C	510	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
23	a	404	PHO	CBC-CAC-C3C	-3.44	107.94	112.87
34	e	101	HEM	CBD-CAD-C3D	-3.44	103.02	112.53
30	c	517	DGD	O6E-C5E-C4E	3.44	115.89	109.70
29	F	102	SQD	C1-O5-C5	-3.43	107.02	113.72
22	b	613	CLA	CMB-C2B-C1B	-3.43	120.20	125.42
30	C	515	DGD	O1G-C1A-C2A	-3.42	101.39	111.83
24	K	102	BCR	C27-C26-C25	3.42	127.32	122.70
24	T	101	BCR	C2-C1-C6	3.41	115.40	110.44
22	C	501	CLA	C4A-NA-C1A	3.41	108.23	106.68
22	B	612	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
26	A	409	PL9	C7-C3-C4	3.40	119.71	116.91
22	B	605	CLA	C4-C3-C5	3.39	121.12	115.23
23	A	404	PHO	C3B-C4B-NB	-3.38	105.26	107.46
27	b	622	LMG	O1-C1-C2	-3.38	103.14	108.27
24	T	101	BCR	C31-C1-C6	3.37	115.53	110.24
22	b	616	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
29	L	101	SQD	O48-C23-C24	3.36	122.09	111.83
23	a	404	PHO	CMB-C2B-C3B	3.36	131.39	124.68
30	h	101	DGD	O3G-C3G-C2G	-3.35	102.66	110.82
22	c	513	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
22	d	402	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
22	D	404	CLA	CHB-C4A-NA	3.35	129.23	124.40
27	d	409	LMG	O6-C1-O1	-3.34	102.16	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	411	CLA	CHD-C1D-ND	-3.33	120.11	124.80
29	L	101	SQD	C3-C4-C5	3.33	116.27	110.23
23	D	401	PHO	C1-C2-C3	-3.33	120.74	126.20
22	B	602	CLA	C3B-C4B-NB	-3.33	107.56	110.53
22	b	605	CLA	C4-C3-C5	3.32	121.00	115.23
30	c	516	DGD	O2E-C2E-C1E	-3.32	102.16	110.08
22	c	502	CLA	C3B-C4B-NB	-3.32	107.57	110.53
35	V	201	HEC	CMC-C2C-C1C	-3.32	120.36	125.42
24	B	617	BCR	C2-C1-C6	3.32	115.26	110.44
22	a	403	CLA	CHB-C4A-NA	3.31	129.18	124.40
24	c	514	BCR	C2-C1-C6	3.31	115.25	110.44
24	B	619	BCR	C29-C30-C25	3.31	115.24	110.44
24	B	617	BCR	C27-C26-C25	3.30	127.16	122.70
22	c	513	CLA	CHB-C4A-NA	3.30	129.16	124.40
24	C	514	BCR	C15-C16-C17	-3.29	116.78	123.52
32	C	519	STE	O2-C1-C2	3.29	124.39	114.00
22	A	403	CLA	C4A-NA-C1A	3.29	108.18	106.68
22	C	513	CLA	C4A-NA-C1A	3.29	108.18	106.68
22	a	411	CLA	O2D-CGD-CBD	3.27	116.94	111.23
22	C	512	CLA	C1-C2-C3	-3.26	120.86	126.20
22	b	602	CLA	C1-C2-C3	-3.26	120.86	126.20
23	a	404	PHO	O2D-CGD-CBD	3.26	114.52	110.95
22	b	601	CLA	C3B-C4B-NB	-3.25	107.63	110.53
22	B	610	CLA	O2A-CGA-O1A	-3.25	115.49	123.63
22	B	614	CLA	C4-C3-C5	3.25	120.86	115.23
26	D	407	PL9	C20-C19-C21	3.25	120.86	115.23
26	d	405	PL9	C7-C3-C2	-3.25	119.56	123.39
22	b	606	CLA	O2D-CGD-CBD	3.25	116.90	111.23
22	B	613	CLA	CMB-C2B-C1B	-3.24	120.48	125.42
22	C	501	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
29	a	412	SQD	O47-C7-C8	3.24	118.49	111.48
22	D	405	CLA	O2D-CGD-CBD	3.24	116.89	111.23
22	B	604	CLA	C1C-C2C-C3C	-3.24	103.58	106.98
24	H	101	BCR	C36-C18-C17	-3.24	117.57	122.82
22	B	613	CLA	C4-C3-C5	3.23	120.84	115.23
24	D	406	BCR	C38-C26-C25	-3.23	120.96	124.48
22	b	612	CLA	CAC-C3C-C4C	3.23	128.99	124.79
24	Z	101	BCR	C11-C10-C9	-3.23	122.75	127.28
27	b	622	LMG	O2-C2-C1	-3.23	102.39	110.08
30	C	515	DGD	O2D-C2D-C1D	-3.23	102.39	110.08
22	C	509	CLA	CHB-C4A-NA	3.22	129.05	124.40
22	b	603	CLA	C4-C3-C5	3.21	120.81	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	PL9	C36-C34-C33	-3.21	113.96	121.17
27	d	409	LMG	O2-C2-C1	-3.21	102.42	110.08
27	b	622	LMG	O6-C5-C6	3.21	114.39	106.44
22	a	403	CLA	C1D-ND-C4D	3.21	108.56	106.31
30	C	517	DGD	O6D-C1D-O3G	-3.20	102.47	110.04
22	C	501	CLA	O2A-CGA-O1A	-3.20	115.63	123.63
26	A	409	PL9	C27-C28-C29	-3.19	120.31	127.62
24	c	514	BCR	C27-C26-C25	3.19	127.02	122.70
22	b	608	CLA	CHB-C4A-NA	3.19	129.01	124.40
29	L	101	SQD	O9-S-O7	-3.19	103.45	113.82
22	C	509	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
30	C	516	DGD	O3G-C1D-C2D	-3.19	103.43	108.27
30	C	517	DGD	O3E-C3E-C2E	-3.19	102.87	110.38
26	a	410	PL9	C20-C19-C21	3.18	120.75	115.23
26	D	407	PL9	C40-C39-C41	3.18	120.75	115.23
22	c	505	CLA	CHB-C4A-NA	3.18	128.99	124.40
22	b	605	CLA	C1-C2-C3	-3.18	120.99	126.20
22	c	513	CLA	C3B-C4B-NB	-3.18	107.69	110.53
29	A	413	SQD	O47-C45-C44	3.18	115.08	107.96
22	C	512	CLA	O2A-CGA-O1A	-3.18	115.68	123.63
22	B	608	CLA	O2D-CGD-CBD	3.17	116.77	111.23
22	C	507	CLA	CHB-C4A-NA	3.17	128.97	124.40
22	B	612	CLA	C3B-C4B-NB	-3.17	107.70	110.53
35	v	201	HEC	C4D-ND-C1D	3.17	110.98	105.82
22	c	502	CLA	C4A-NA-C1A	3.15	108.12	106.68
22	B	607	CLA	CHB-C4A-NA	3.14	128.94	124.40
24	A	406	BCR	C27-C26-C25	3.14	126.95	122.70
22	c	504	CLA	CMB-C2B-C1B	-3.14	120.64	125.42
24	H	101	BCR	C27-C26-C25	3.14	126.94	122.70
23	D	401	PHO	C2B-C1B-NB	-3.14	107.16	109.43
29	A	412	SQD	O9-S-O7	-3.13	103.63	113.82
22	b	608	CLA	O2D-CGD-CBD	3.13	116.70	111.23
26	d	405	PL9	C37-C38-C39	-3.13	120.46	127.62
22	B	610	CLA	CHB-C4A-NA	3.13	128.92	124.40
24	d	404	BCR	C27-C26-C25	3.13	126.93	122.70
22	c	512	CLA	C3B-C4B-NB	-3.13	107.74	110.53
22	b	602	CLA	O2D-CGD-CBD	3.12	116.69	111.23
22	c	501	CLA	CED-O2D-CGD	-3.12	108.83	115.92
22	b	612	CLA	C4A-NA-C1A	3.12	108.10	106.68
34	F	101	HEM	CHC-C4B-NB	3.12	127.78	124.42
22	a	403	CLA	C2D-C1D-ND	-3.12	107.04	110.13
22	B	615	CLA	CHB-C4A-NA	3.12	128.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	C6-C5-C3	-3.11	105.89	113.47
27	a	414	LMG	O6-C1-O1	-3.11	102.71	110.04
23	A	404	PHO	O2D-CGD-CBD	3.10	114.35	110.95
24	t	101	BCR	C7-C8-C9	-3.09	121.66	126.23
22	C	501	CLA	C3B-C4B-NB	-3.09	107.77	110.53
30	c	515	DGD	O6D-C1D-O3G	-3.08	102.76	110.04
22	c	511	CLA	C3B-C4B-NB	-3.08	107.78	110.53
30	h	101	DGD	C4E-C3E-C2E	-3.08	105.43	110.83
22	B	612	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
22	B	602	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
26	D	407	PL9	C37-C38-C39	-3.08	120.58	127.62
23	d	401	PHO	C1-C2-C3	-3.07	121.16	126.20
22	a	402	CLA	O2A-CGA-O1A	-3.07	115.95	123.63
24	K	102	BCR	C37-C22-C21	-3.06	117.85	122.82
22	c	501	CLA	O2A-CGA-O1A	-3.06	115.97	123.63
32	x	102	STE	O2-C1-C2	3.06	123.67	114.00
22	B	615	CLA	C3B-C4B-NB	-3.05	107.81	110.53
22	b	610	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
22	c	501	CLA	O2D-CGD-CBD	3.05	116.56	111.23
22	B	607	CLA	O2A-CGA-O1A	-3.04	116.02	123.63
23	A	404	PHO	OBD-CAD-CBD	-3.04	121.36	125.82
33	a	409	BCT	O3-C-O1	-3.04	111.90	119.68
29	a	412	SQD	O47-C7-O49	-3.04	116.60	123.70
22	b	602	CLA	C3B-C4B-NB	-3.03	107.82	110.53
22	B	602	CLA	O2D-CGD-CBD	3.03	116.53	111.23
24	T	101	BCR	C27-C26-C25	3.03	126.80	122.70
27	m	101	LMG	O7-C10-O9	-3.03	116.62	123.70
22	C	511	CLA	C1-C2-C3	-3.03	121.23	126.20
22	b	613	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
22	b	609	CLA	O1D-CGD-CBD	3.02	130.48	124.52
30	c	517	DGD	O6D-C1D-O3G	-3.02	102.90	110.04
26	d	405	PL9	C22-C23-C24	-3.02	120.71	127.62
22	B	604	CLA	C1-O2A-CGA	-3.02	109.34	116.65
27	a	414	LMG	C1-O6-C5	-3.02	107.82	113.72
24	T	101	BCR	C7-C8-C9	-3.02	121.77	126.23
22	B	615	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
30	H	102	DGD	O6D-C1D-O3G	-3.00	102.95	110.04
28	d	407	LHG	O8-C23-O10	-2.99	116.15	123.63
22	a	403	CLA	O2D-CGD-CBD	2.99	116.45	111.23
22	B	604	CLA	C2C-C1C-NC	2.99	113.12	109.98
28	A	411	LHG	O8-C23-C24	2.99	120.94	111.83
29	f	101	SQD	C1-C2-C3	-2.98	103.73	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	CLA	O2D-CGD-CBD	2.98	116.44	111.23
22	B	603	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
27	m	101	LMG	C1-O6-C5	-2.98	107.90	113.72
22	A	402	CLA	C4A-NA-C1A	2.98	108.04	106.68
22	c	502	CLA	CHD-C1D-ND	-2.98	120.61	124.80
29	a	413	SQD	O49-C7-C8	-2.98	112.14	123.78
22	d	402	CLA	C3B-C4B-NB	-2.98	107.87	110.53
24	Z	101	BCR	C7-C8-C9	-2.98	121.83	126.23
22	B	603	CLA	C3B-C4B-NB	-2.97	107.88	110.53
29	B	622	SQD	C1-C2-C3	-2.97	103.76	110.01
24	t	101	BCR	C1-C6-C5	-2.97	118.58	122.64
22	c	502	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	B	606	CLA	O2D-CGD-CBD	2.96	116.41	111.23
22	A	402	CLA	CAC-C3C-C4C	2.96	128.64	124.79
24	B	618	BCR	C15-C16-C17	-2.96	117.46	123.52
22	b	603	CLA	CMB-C2B-C3B	2.96	133.51	126.55
26	d	405	PL9	C35-C34-C36	2.96	120.36	115.23
22	B	609	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
22	b	610	CLA	CHB-C4A-NA	2.96	128.66	124.40
29	A	413	SQD	O47-C7-C8	2.95	117.87	111.48
22	d	402	CLA	O1D-CGD-CBD	2.95	130.34	124.52
24	b	618	BCR	C36-C18-C17	-2.95	118.03	122.82
22	B	606	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
24	Z	101	BCR	C15-C14-C13	-2.95	123.14	127.28
29	a	413	SQD	O48-C23-C24	2.95	120.82	111.83
24	A	406	BCR	C15-C16-C17	-2.95	117.49	123.52
30	c	516	DGD	O3G-C3G-C2G	-2.94	103.66	110.82
29	L	101	SQD	O2-C2-C1	2.94	117.08	110.08
29	a	413	SQD	O48-C23-O10	-2.94	116.28	123.63
22	a	411	CLA	CHD-C1D-C2D	2.94	131.59	125.49
22	a	405	CLA	CHB-C4A-NA	2.94	128.64	124.40
24	k	102	BCR	C27-C26-C25	2.93	126.67	122.70
22	C	504	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
27	M	101	LMG	O6-C1-O1	-2.93	103.12	110.04
27	c	518	LMG	C9-C8-C7	-2.93	104.95	111.78
22	B	612	CLA	C11-C12-C13	-2.92	106.24	115.97
29	a	412	SQD	O9-S-O7	-2.92	104.32	113.82
22	d	403	CLA	CMB-C2B-C1B	-2.92	120.98	125.42
28	D	409	LHG	O8-C23-C24	2.92	120.72	111.83
22	B	612	CLA	O1D-CGD-CBD	2.91	130.26	124.52
26	A	409	PL9	C41-C39-C38	-2.91	114.63	121.17
22	b	616	CLA	O1D-CGD-CBD	2.90	130.25	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	O2D-CGD-CBD	2.90	116.31	111.23
22	b	614	CLA	CHB-C4A-NA	2.90	128.59	124.40
30	C	515	DGD	O3E-C3E-C2E	-2.90	103.55	110.38
24	Z	101	BCR	C2-C1-C6	2.89	114.64	110.44
22	C	505	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
22	B	604	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
22	b	608	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	B	608	CLA	C3B-C4B-NB	-2.89	107.95	110.53
29	a	412	SQD	O48-C23-C24	2.89	120.63	111.83
22	C	505	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
26	a	410	PL9	C37-C38-C39	-2.88	121.04	127.62
26	a	410	PL9	C27-C28-C29	-2.88	121.04	127.62
26	a	410	PL9	C25-C24-C26	2.88	120.22	115.23
22	B	607	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
30	c	516	DGD	O3G-C1D-C2D	-2.87	103.91	108.27
24	D	406	BCR	C27-C26-C25	2.87	126.58	122.70
22	B	614	CLA	O1D-CGD-CBD	2.87	130.18	124.52
22	c	508	CLA	CMB-C2B-C3B	2.87	133.29	126.55
30	A	414	DGD	C3G-C2G-C1G	-2.87	105.10	111.78
22	b	602	CLA	CHB-C4A-NA	2.86	128.53	124.40
22	B	604	CLA	C6-C5-C3	-2.86	106.50	113.47
22	B	605	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
22	b	614	CLA	C1-C2-C3	-2.86	121.51	126.20
22	b	610	CLA	CAA-CBA-CGA	-2.86	105.10	113.21
30	C	516	DGD	O5D-C6D-C5D	-2.86	102.98	109.42
29	A	412	SQD	C1-O5-C5	-2.85	108.15	113.72
22	B	607	CLA	C3B-C4B-NB	-2.85	107.99	110.53
29	L	101	SQD	O5-C5-C4	2.85	114.83	109.70
28	E	101	LHG	O8-C23-C24	2.85	120.51	111.83
27	a	414	LMG	O8-C28-O10	-2.84	116.53	123.63
30	c	515	DGD	O4D-C4D-C5D	-2.84	102.34	109.32
26	D	407	PL9	C35-C34-C36	2.84	120.15	115.23
22	B	615	CLA	CHC-C4B-NB	2.83	128.30	124.05
30	A	414	DGD	CDB-CCB-CBB	-2.83	100.06	114.37
22	C	503	CLA	C7-C6-C5	-2.83	105.72	113.26
26	A	409	PL9	O1-C4-C3	-2.83	117.75	120.73
24	C	514	BCR	C27-C26-C25	2.82	126.52	122.70
22	B	610	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
30	A	414	DGD	O1G-C1A-O1A	-2.82	116.57	123.63
22	c	508	CLA	CHD-C1D-ND	-2.82	120.83	124.80
22	C	503	CLA	O2A-CGA-O1A	-2.82	116.57	123.63
26	A	409	PL9	C40-C39-C38	-2.82	116.39	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CHB-C4A-NA	2.81	128.46	124.40
29	A	412	SQD	O5-C1-C2	-2.81	104.59	110.37
26	d	405	PL9	C36-C34-C33	-2.81	114.86	121.17
22	C	506	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
27	C	518	LMG	O2-C2-C1	-2.81	103.38	110.08
22	B	608	CLA	CHB-C1B-NB	2.81	128.26	124.05
24	C	514	BCR	C38-C26-C25	-2.80	121.43	124.48
22	c	510	CLA	O1D-CGD-CBD	2.80	130.03	124.52
22	a	405	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
22	B	604	CLA	O2D-CGD-CBD	2.79	116.11	111.23
22	B	616	CLA	CAA-CBA-CGA	-2.79	105.28	113.21
22	d	403	CLA	C4A-NA-C1A	2.79	107.95	106.68
24	b	619	BCR	C2-C1-C6	2.79	114.50	110.44
22	A	403	CLA	O2D-CGD-CBD	2.79	116.11	111.23
29	a	412	SQD	C1-C2-C3	-2.79	104.14	110.01
28	D	409	LHG	O7-C7-C8	-2.79	105.44	111.48
22	b	603	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
30	c	517	DGD	O5E-C6E-C5E	-2.78	101.85	111.33
30	h	101	DGD	O6D-C1D-O3G	-2.78	103.47	110.04
22	c	513	CLA	CAC-C3C-C4C	2.78	128.41	124.79
22	a	403	CLA	CHD-C1D-C2D	2.78	131.26	125.49
22	C	512	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	k	102	BCR	C38-C26-C25	-2.77	121.47	124.48
24	x	101	BCR	C27-C26-C25	2.76	126.44	122.70
22	D	403	CLA	C3B-C4B-NB	-2.76	108.06	110.53
30	H	102	DGD	C6D-C5D-C4D	2.76	117.86	112.07
22	B	611	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
22	b	613	CLA	O2A-CGA-O1A	-2.76	116.73	123.63
29	B	622	SQD	O5-C5-C4	2.76	114.67	109.70
30	B	623	DGD	O3G-C3G-C2G	-2.75	104.70	111.77
22	b	603	CLA	CHB-C1B-NB	2.75	128.18	124.05
26	a	410	PL9	C22-C23-C24	-2.75	121.33	127.62
24	c	514	BCR	C38-C26-C25	-2.75	121.48	124.48
22	B	611	CLA	C3B-C4B-NB	-2.75	108.08	110.53
22	B	612	CLA	C1-C2-C3	-2.74	121.70	126.20
35	V	201	HEC	CHD-C4C-NC	2.74	127.44	124.45
22	B	612	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
30	C	515	DGD	O5D-C6D-C5D	-2.73	103.26	109.42
27	m	101	LMG	C9-C8-C7	-2.73	105.41	111.78
30	c	515	DGD	O3G-C3G-C2G	-2.73	104.17	110.82
22	B	602	CLA	C4A-NA-C1A	2.73	107.92	106.68
35	V	201	HEC	CMB-C2B-C1B	-2.73	121.26	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	621	LHG	C11-C10-C9	-2.73	100.58	114.37
24	K	101	BCR	C15-C16-C17	-2.73	117.94	123.52
22	B	601	CLA	C3B-C4B-NB	-2.73	108.10	110.53
22	D	405	CLA	CHC-C4B-NB	2.72	128.13	124.05
24	B	619	BCR	C1-C6-C5	-2.72	118.91	122.64
34	e	101	HEM	C3B-C2B-C1B	2.72	108.45	106.41
26	a	410	PL9	C26-C24-C23	-2.72	115.06	121.17
27	d	409	LMG	C40-C39-C38	-2.72	100.61	114.37
23	D	401	PHO	O2D-CGD-O1D	-2.72	118.56	123.85
22	C	510	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
22	b	604	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	b	605	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	c	511	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
29	f	101	SQD	O9-S-C6	2.71	110.81	106.76
22	c	509	CLA	CHD-C1D-ND	-2.71	120.99	124.80
22	C	502	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	b	612	CLA	CHB-C4A-NA	2.70	128.30	124.40
24	b	617	BCR	C27-C26-C25	2.70	126.36	122.70
22	a	402	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	c	504	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
22	c	512	CLA	O1D-CGD-CBD	2.70	129.84	124.52
26	A	409	PL9	C7-C3-C2	-2.70	120.21	123.39
24	K	102	BCR	C2-C1-C6	2.70	114.36	110.44
22	C	501	CLA	C2D-C1D-ND	-2.70	107.46	110.13
22	C	512	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
22	C	513	CLA	O2A-CGA-O1A	-2.69	116.89	123.63
22	C	504	CLA	CED-O2D-CGD	2.69	122.02	115.92
22	c	507	CLA	CHD-C4C-NC	2.69	128.40	124.23
32	C	519	STE	O2-C1-O1	-2.69	116.42	123.33
22	B	611	CLA	C1-C2-C3	-2.69	121.79	126.20
22	B	609	CLA	O2A-CGA-O1A	-2.69	116.91	123.63
29	F	102	SQD	O48-C23-O10	-2.69	116.91	123.63
26	A	409	PL9	O2-C1-C6	2.68	124.75	120.48
22	B	616	CLA	CHB-C4A-NA	2.68	128.27	124.40
29	B	622	SQD	O48-C23-O10	-2.68	116.92	123.63
22	B	604	CLA	CHB-C4A-NA	2.68	128.27	124.40
22	B	608	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
24	c	514	BCR	C36-C18-C17	-2.68	118.48	122.82
22	a	402	CLA	O1D-CGD-CBD	2.67	129.78	124.52
24	Z	101	BCR	C36-C18-C17	-2.67	118.49	122.82
22	C	513	CLA	O1D-CGD-CBD	2.67	129.78	124.52
28	d	406	LHG	C5-O7-C7	-2.67	111.41	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	BCR	C15-C16-C17	-2.67	118.06	123.52
30	c	516	DGD	O6D-C1D-O3G	-2.66	103.75	110.04
32	M	102	STE	O2-C1-C2	2.66	122.41	114.00
22	B	610	CLA	C1-C2-C3	-2.66	121.84	126.20
24	k	101	BCR	C38-C26-C25	-2.66	121.58	124.48
29	L	101	SQD	C45-O47-C7	2.66	124.16	117.80
22	B	615	CLA	C2A-C3A-C4A	2.66	106.16	101.87
30	c	516	DGD	O3D-C3D-C4D	-2.66	104.11	110.38
27	M	101	LMG	C38-C37-C36	-2.66	100.94	114.37
26	d	405	PL9	C20-C19-C21	2.66	119.84	115.23
26	a	410	PL9	O2-C1-C6	2.65	124.70	120.48
22	c	504	CLA	CHD-C1D-ND	-2.65	121.07	124.80
27	D	408	LMG	O2-C2-C1	-2.65	103.76	110.08
22	b	609	CLA	CMB-C2B-C3B	2.65	132.78	126.55
27	b	622	LMG	C3-C4-C5	-2.65	105.43	110.23
22	B	606	CLA	C7-C6-C5	-2.64	106.22	113.26
22	B	614	CLA	CHC-C4B-NB	2.64	128.01	124.05
27	d	409	LMG	O1-C1-C2	-2.64	104.26	108.27
24	K	101	BCR	C38-C26-C25	-2.64	121.60	124.48
29	L	101	SQD	O47-C7-O49	-2.64	117.53	123.70
22	A	405	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
22	b	614	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
26	D	407	PL9	C42-C43-C44	-2.64	121.58	127.62
24	K	101	BCR	C27-C26-C25	2.64	126.27	122.70
22	b	610	CLA	C2C-C1C-NC	2.64	112.75	109.98
22	C	506	CLA	C3B-C4B-NB	-2.63	108.18	110.53
32	m	102	STE	O2-C1-C2	2.62	122.29	114.00
27	c	520	LMG	O2-C2-C1	-2.62	103.83	110.08
29	a	412	SQD	C1-O5-C5	-2.62	108.60	113.72
22	D	404	CLA	O2D-CGD-CBD	2.62	115.80	111.23
22	b	616	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
22	b	607	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
23	a	404	PHO	O2D-CGD-O1D	-2.61	118.76	123.85
28	b	623	LHG	O2-C2-C3	-2.61	100.67	109.70
28	b	623	LHG	O8-C23-C24	2.61	119.79	111.83
22	c	507	CLA	CHD-C1D-ND	-2.61	121.13	124.80
30	c	516	DGD	C3E-C4E-C5E	-2.61	105.50	110.23
27	m	101	LMG	O8-C28-O10	-2.61	117.10	123.63
24	b	619	BCR	C37-C22-C21	-2.61	118.59	122.82
22	B	612	CLA	CMB-C2B-C3B	2.61	132.68	126.55
30	C	515	DGD	C3G-C2G-C1G	-2.60	105.72	111.78
22	b	615	CLA	CHB-C1B-NB	2.60	127.95	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	409	LHG	O8-C23-O10	-2.60	117.12	123.63
22	B	616	CLA	C3B-C4B-NB	-2.60	108.21	110.53
23	a	404	PHO	C3B-C4B-NB	-2.60	105.77	107.46
27	c	518	LMG	O3-C3-C2	-2.60	104.25	110.38
22	B	611	CLA	O2D-CGD-CBD	2.60	115.77	111.23
32	J	101	STE	O2-C1-C2	2.60	122.20	114.00
22	b	616	CLA	CMB-C2B-C3B	2.60	132.66	126.55
22	D	403	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	x	101	BCR	C36-C18-C17	-2.59	118.61	122.82
22	B	602	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
24	k	103	BCR	C29-C30-C25	2.59	114.20	110.44
32	C	521	STE	O2-C1-C2	2.59	122.18	114.00
22	C	508	CLA	C3B-C4B-NB	-2.59	108.22	110.53
27	d	409	LMG	O6-C5-C4	2.59	114.36	109.70
29	B	622	SQD	C46-C45-C44	-2.58	105.76	111.78
22	a	405	CLA	O2D-CGD-CBD	2.58	115.74	111.23
22	C	505	CLA	CMB-C2B-C3B	2.58	132.62	126.55
22	b	611	CLA	CHB-C1B-NB	2.58	127.92	124.05
29	a	412	SQD	O8-S-C6	2.58	110.95	105.97
35	V	201	HEC	CHB-C4A-NA	2.58	127.26	124.45
22	c	510	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
22	c	502	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
24	b	618	BCR	C30-C25-C26	-2.57	119.12	122.64
22	B	611	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
30	C	515	DGD	O6D-C1D-O3G	-2.57	103.97	110.04
22	B	613	CLA	CMB-C2B-C3B	2.57	132.59	126.55
22	c	503	CLA	C4-C3-C5	2.57	119.69	115.23
22	b	612	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
22	b	605	CLA	O1D-CGD-CBD	2.57	129.58	124.52
24	x	101	BCR	C2-C1-C6	2.56	114.16	110.44
22	A	402	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
22	C	513	CLA	O2D-CGD-CBD	2.56	115.71	111.23
22	c	502	CLA	CMB-C2B-C3B	2.56	132.56	126.55
30	c	516	DGD	C6D-O5D-C1E	2.55	119.27	113.80
24	k	103	BCR	C27-C26-C25	2.55	126.16	122.70
24	B	617	BCR	C30-C25-C26	-2.55	119.15	122.64
23	A	404	PHO	C1A-C2A-C3A	-2.55	100.41	102.84
22	C	506	CLA	O1D-CGD-CBD	2.55	129.55	124.52
22	c	506	CLA	C3B-C4B-NB	-2.55	108.25	110.53
22	c	504	CLA	CHB-C4A-NA	2.55	128.08	124.40
22	B	605	CLA	C4-C3-C2	-2.54	117.10	123.63
24	k	103	BCR	C37-C22-C21	-2.54	118.70	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	CHB-C4A-NA	2.54	128.07	124.40
22	d	403	CLA	CMB-C2B-C3B	2.54	132.52	126.55
22	a	402	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
23	D	401	PHO	CMB-C2B-C3B	2.54	129.75	124.68
32	k	104	STE	O2-C1-C2	2.53	122.01	114.00
22	A	403	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
22	B	602	CLA	CMB-C2B-C3B	2.53	132.50	126.55
22	B	608	CLA	C6-C7-C8	-2.53	107.56	115.97
24	A	406	BCR	C16-C15-C14	-2.53	118.34	123.52
22	b	604	CLA	CHB-C4A-NA	2.53	128.05	124.40
35	V	201	HEC	C4D-ND-C1D	2.53	109.94	105.82
22	C	513	CLA	CHB-C4A-NA	2.53	128.05	124.40
23	d	401	PHO	CBA-CAA-C2A	-2.53	106.34	113.78
30	h	101	DGD	C3D-C4D-C5D	-2.52	105.66	110.23
22	C	509	CLA	CMB-C2B-C3B	2.52	132.49	126.55
22	c	508	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	D	401	PHO	OBD-CAD-CBD	-2.52	122.12	125.82
22	B	604	CLA	CMB-C2B-C3B	2.52	132.48	126.55
24	k	101	BCR	C27-C26-C25	2.52	126.11	122.70
32	c	519	STE	O2-C1-C2	2.52	121.96	114.00
26	a	410	PL9	O2-C1-C2	-2.52	116.10	121.83
24	K	102	BCR	C40-C30-C25	2.52	114.19	110.24
30	C	516	DGD	C4E-C3E-C2E	-2.51	106.42	110.83
23	A	404	PHO	O2A-CGA-O1A	-2.51	117.34	123.63
22	B	606	CLA	CHB-C4A-NA	2.51	128.03	124.40
30	c	517	DGD	CDB-CCB-CBB	-2.51	101.68	114.37
30	c	517	DGD	O6E-C1E-O5D	-2.51	104.12	110.04
27	M	101	LMG	O7-C10-O9	-2.51	117.85	123.70
26	D	407	PL9	C7-C8-C9	-2.51	122.52	126.83
22	B	607	CLA	CAC-C3C-C4C	2.50	128.05	124.79
22	C	504	CLA	C4-C3-C5	2.50	119.58	115.23
22	C	511	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
22	b	602	CLA	O1D-CGD-CBD	2.50	129.46	124.52
23	d	401	PHO	O2D-CGD-O1D	-2.50	118.98	123.85
28	l	101	LHG	O8-C23-C24	2.50	119.46	111.83
28	e	102	LHG	C11-C10-C9	-2.50	101.72	114.37
24	T	101	BCR	C3-C4-C5	-2.50	109.60	114.06
29	A	412	SQD	O47-C7-O49	-2.50	117.86	123.70
22	B	603	CLA	O1D-CGD-CBD	2.50	129.45	124.52
22	a	403	CLA	C3C-C4C-NC	-2.50	107.23	110.43
22	C	503	CLA	O1D-CGD-CBD	2.50	129.44	124.52
24	k	101	BCR	C15-C16-C17	-2.49	118.41	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	515	DGD	C3E-C4E-C5E	-2.49	105.71	110.23
27	C	518	LMG	C38-C37-C36	-2.49	101.76	114.37
22	B	614	CLA	O2D-CGD-CBD	2.49	115.59	111.23
22	B	611	CLA	CHB-C4A-NA	2.49	128.00	124.40
23	A	404	PHO	CMB-C2B-C3B	2.49	129.66	124.68
22	B	603	CLA	C2D-C1D-ND	-2.49	107.66	110.13
22	c	512	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
22	D	405	CLA	CMB-C2B-C3B	2.49	132.40	126.55
28	D	409	LHG	C20-C19-C18	-2.49	101.79	114.37
29	B	622	SQD	O8-S-C6	2.49	110.77	105.97
29	L	101	SQD	O5-C1-C2	-2.49	105.26	110.37
22	b	609	CLA	CED-O2D-CGD	2.48	121.55	115.92
22	A	405	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
27	C	518	LMG	O7-C10-O9	-2.48	117.91	123.70
22	D	405	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
22	b	607	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	d	404	BCR	C30-C25-C26	-2.48	119.25	122.64
30	C	516	DGD	C5B-C4B-C3B	-2.47	101.88	114.37
22	a	403	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
30	C	516	DGD	C6D-O5D-C1E	2.47	119.09	113.80
22	C	511	CLA	O2D-CGD-CBD	2.46	115.53	111.23
24	k	102	BCR	C36-C18-C17	-2.46	118.83	122.82
35	v	201	HEC	CHD-C1D-ND	2.46	128.32	123.86
22	b	607	CLA	CHB-C1B-NB	2.46	127.74	124.05
24	A	406	BCR	C36-C18-C17	-2.46	118.83	122.82
28	B	621	LHG	O8-C23-C24	2.46	119.32	111.83
24	c	514	BCR	C15-C16-C17	-2.46	118.50	123.52
22	a	402	CLA	CAC-C3C-C4C	2.46	127.98	124.79
30	C	516	DGD	C3E-C4E-C5E	-2.45	105.78	110.23
24	B	619	BCR	C37-C22-C21	-2.45	118.84	122.82
29	F	102	SQD	O2-C2-C3	2.45	116.16	110.38
28	l	101	LHG	C27-C26-C25	-2.45	101.96	114.37
30	C	516	DGD	O3E-C3E-C2E	-2.45	104.60	110.38
22	C	506	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
22	B	603	CLA	CHD-C4C-NC	2.45	128.03	124.23
22	B	609	CLA	C2C-C1C-NC	2.45	112.55	109.98
24	d	404	BCR	C2-C1-C6	2.44	113.99	110.44
27	C	518	LMG	O1-C7-C8	-2.44	104.87	110.82
30	c	516	DGD	CDB-CCB-CBB	-2.44	102.03	114.37
26	A	409	PL9	C35-C34-C36	2.44	119.46	115.23
22	b	603	CLA	CHD-C1D-C2D	2.44	130.56	125.49
22	B	614	CLA	C6-C5-C3	2.44	119.41	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	PL9	O2-C1-C2	-2.44	116.29	121.83
27	c	518	LMG	O1-C7-C8	-2.44	104.89	110.82
22	c	508	CLA	C3B-C4B-NB	-2.44	108.36	110.53
27	b	622	LMG	O7-C10-O9	-2.43	118.02	123.70
22	b	610	CLA	C3B-C4B-NB	-2.43	108.36	110.53
27	D	408	LMG	C3-C4-C5	-2.43	105.83	110.23
22	c	512	CLA	CHC-C1C-NC	2.43	127.97	124.31
22	c	508	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
24	b	619	BCR	C27-C26-C25	2.43	125.98	122.70
27	c	520	LMG	O1-C1-C2	-2.43	104.59	108.27
22	c	504	CLA	O2D-CGD-CBD	2.42	115.47	111.23
22	c	507	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
27	c	520	LMG	C6-C5-C4	-2.42	107.07	113.02
22	c	508	CLA	CGD-CBD-CAD	-2.42	103.00	110.85
22	B	609	CLA	CHA-C1A-NA	-2.42	120.91	126.39
30	h	101	DGD	C3G-C2G-C1G	-2.42	106.14	111.78
22	c	510	CLA	CHB-C1B-NB	2.42	127.68	124.05
27	m	101	LMG	C38-C37-C36	-2.42	102.14	114.37
22	b	612	CLA	CMB-C2B-C3B	2.42	132.24	126.55
27	a	414	LMG	O5-C6-C5	-2.42	103.10	111.33
22	b	613	CLA	CMB-C2B-C3B	2.42	132.23	126.55
24	x	101	BCR	C11-C10-C9	-2.41	123.89	127.28
22	b	603	CLA	CHB-C1B-C2B	-2.41	120.43	127.43
22	B	603	CLA	C16-C15-C13	-2.41	107.95	115.97
28	b	623	LHG	C11-C10-C9	-2.41	102.18	114.37
28	B	621	LHG	O8-C23-O10	-2.41	117.60	123.63
22	A	403	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
27	D	411	LMG	O8-C28-O10	-2.41	117.14	123.33
30	c	516	DGD	O2D-C2D-C1D	-2.41	104.34	110.08
22	D	405	CLA	C3B-C4B-NB	-2.41	108.38	110.53
30	B	623	DGD	CFB-CEB-CDB	-2.41	102.21	114.37
24	b	618	BCR	C39-C30-C25	-2.40	106.47	110.24
24	A	406	BCR	C2-C1-C6	2.40	113.93	110.44
22	c	505	CLA	O2D-CGD-CBD	2.40	115.43	111.23
24	a	406	BCR	C33-C5-C6	-2.40	121.86	124.48
30	C	516	DGD	O6D-C1D-O3G	-2.40	104.37	110.04
22	B	607	CLA	C2A-C1A-CHA	2.40	128.03	123.87
34	e	101	HEM	CAB-C3B-C2B	-2.40	120.63	128.43
26	D	407	PL9	O2-C1-C2	-2.40	116.37	121.83
35	V	201	HEC	CBD-CAD-C3D	-2.40	105.91	112.53
22	b	616	CLA	CHC-C4B-NB	2.40	127.64	124.05
27	m	101	LMG	O1-C7-C8	-2.40	104.99	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	C7-C6-C5	-2.39	106.88	113.26
24	a	406	BCR	C27-C26-C25	2.39	125.94	122.70
30	C	516	DGD	CDB-CCB-CBB	-2.39	102.27	114.37
29	F	102	SQD	C46-C45-C44	-2.39	105.94	113.67
22	b	604	CLA	CHC-C1C-NC	2.39	127.91	124.31
24	x	101	BCR	C37-C22-C21	-2.39	118.95	122.82
24	b	618	BCR	C27-C26-C25	2.38	125.93	122.70
24	B	617	BCR	C38-C26-C25	-2.38	121.88	124.48
29	F	102	SQD	O5-C5-C4	2.38	113.99	109.70
26	a	410	PL9	C21-C19-C18	-2.38	115.82	121.17
35	v	201	HEC	CHB-C1B-NB	2.38	128.18	123.86
22	C	513	CLA	CHD-C1D-ND	-2.38	121.45	124.80
24	Z	101	BCR	C36-C18-C19	2.38	121.73	118.09
29	a	412	SQD	O5-C1-C2	-2.38	105.48	110.37
22	b	605	CLA	C3B-C4B-NB	-2.38	108.40	110.53
28	d	406	LHG	O8-C23-C24	2.38	119.09	111.83
22	c	509	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
22	B	603	CLA	CHB-C4A-NA	2.38	127.83	124.40
22	B	607	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
24	b	617	BCR	C3-C4-C5	-2.37	109.82	114.06
22	b	613	CLA	CAA-CBA-CGA	2.37	119.95	113.21
22	A	405	CLA	C4-C3-C5	2.37	119.35	115.23
24	b	619	BCR	C36-C18-C17	-2.37	118.97	122.82
22	D	404	CLA	CMB-C2B-C3B	2.37	132.13	126.55
22	C	509	CLA	CHD-C1D-ND	-2.37	121.46	124.80
30	C	517	DGD	C8B-C7B-C6B	-2.37	102.38	114.37
22	B	615	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
22	c	512	CLA	C2D-C1D-ND	-2.37	107.78	110.13
26	a	410	PL9	C12-C13-C14	-2.37	122.20	127.62
24	Z	101	BCR	C38-C26-C25	-2.37	121.90	124.48
29	L	101	SQD	O47-C45-C46	2.37	116.84	108.34
22	a	411	CLA	C1-C2-C3	-2.37	122.32	126.20
22	c	510	CLA	C3B-C4B-NB	-2.37	108.42	110.53
22	B	603	CLA	C1D-ND-C4D	2.37	107.97	106.31
26	D	407	PL9	O2-C1-C6	2.37	124.25	120.48
24	H	101	BCR	C29-C30-C25	2.37	113.88	110.44
35	v	201	HEC	CHA-C4D-ND	2.37	128.15	123.86
22	B	602	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
22	B	613	CLA	CHA-C1A-NA	-2.37	121.03	126.39
30	A	414	DGD	CBB-CAB-C9B	-2.36	102.42	114.37
23	a	404	PHO	OBD-CAD-C3D	2.36	131.58	127.89
30	A	414	DGD	O2D-C2D-C1D	-2.36	104.45	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	CHB-C4A-NA	2.36	127.81	124.40
24	d	404	BCR	C24-C23-C22	-2.36	122.74	126.23
22	C	505	CLA	C3B-C4B-NB	-2.36	108.42	110.53
30	c	515	DGD	O3G-C1D-C2D	-2.36	104.69	108.27
22	B	603	CLA	CHD-C1D-C2D	2.36	130.39	125.49
22	B	613	CLA	O1D-CGD-CBD	2.36	129.17	124.52
30	H	102	DGD	C8B-C7B-C6B	-2.36	102.45	114.37
29	L	101	SQD	O10-C23-C24	-2.36	114.57	123.78
22	C	507	CLA	C3B-C4B-NB	-2.36	108.43	110.53
23	D	401	PHO	CMD-C2D-C3D	2.35	129.39	124.68
26	d	405	PL9	C7-C8-C9	-2.35	122.78	126.83
22	b	613	CLA	CED-O2D-CGD	2.35	121.25	115.92
30	H	102	DGD	C1D-C2D-C3D	-2.35	105.07	110.01
24	x	101	BCR	C24-C23-C22	-2.35	122.76	126.23
22	c	503	CLA	CHB-C1B-NB	2.35	127.57	124.05
22	c	507	CLA	C3B-C4B-NB	-2.35	108.44	110.53
22	C	503	CLA	O2A-C1-C2	-2.35	99.08	108.11
24	A	406	BCR	C40-C30-C25	2.34	113.92	110.24
22	A	402	CLA	C3B-C4B-NB	-2.34	108.44	110.53
22	c	501	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	c	511	CLA	CHB-C1B-NB	2.34	127.56	124.05
30	c	515	DGD	O1G-C1A-C2A	-2.34	104.70	111.83
24	B	617	BCR	C23-C22-C21	-2.34	115.33	119.01
22	C	509	CLA	C16-C15-C13	-2.34	108.19	115.97
22	B	608	CLA	CHA-C1A-NA	-2.34	121.10	126.39
22	b	603	CLA	CHD-C1D-ND	-2.34	121.52	124.80
22	C	507	CLA	C1-C2-C3	-2.33	122.38	126.20
24	b	617	BCR	C15-C16-C17	-2.33	118.75	123.52
22	c	510	CLA	CMA-C3A-C2A	-2.33	104.97	113.98
22	B	603	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
22	D	404	CLA	C7-C6-C5	-2.33	107.06	113.26
30	A	414	DGD	C1D-C2D-C3D	-2.33	105.11	110.01
22	b	601	CLA	CHD-C1D-ND	-2.33	121.53	124.80
22	c	502	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
22	B	611	CLA	C2D-C1D-ND	-2.32	107.83	110.13
30	h	101	DGD	C7B-C6B-C5B	-2.32	102.64	114.37
27	c	520	LMG	C9-C8-C7	-2.32	106.37	111.78
22	B	602	CLA	CHD-C1D-ND	-2.32	121.54	124.80
24	D	406	BCR	C2-C1-C6	2.32	113.81	110.44
22	A	403	CLA	C1-C2-C3	-2.32	122.40	126.20
29	B	622	SQD	O48-C23-C24	2.32	118.89	111.83
22	A	403	CLA	CMB-C2B-C3B	2.31	132.00	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	623	LHG	O8-C23-O10	-2.31	117.84	123.63
28	d	406	LHG	C20-C19-C18	-2.31	102.67	114.37
30	h	101	DGD	C1D-C2D-C3D	-2.31	105.14	110.01
29	A	413	SQD	O48-C23-O10	-2.31	117.84	123.63
22	C	501	CLA	CHB-C1B-NB	2.31	127.52	124.05
24	x	101	BCR	C16-C15-C14	-2.31	118.79	123.52
24	b	618	BCR	C36-C18-C19	2.31	121.62	118.09
22	a	405	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
28	E	101	LHG	O8-C23-O10	-2.31	117.85	123.63
22	B	602	CLA	C11-C12-C13	-2.31	108.29	115.97
30	h	101	DGD	O6E-C1E-O5D	-2.31	104.59	110.04
22	B	604	CLA	C16-C15-C13	-2.31	108.30	115.97
26	D	407	PL9	C22-C23-C24	-2.31	122.34	127.62
35	v	201	HEC	CBD-CAD-C3D	-2.31	106.15	112.53
29	A	413	SQD	O49-C7-C8	-2.31	114.76	123.78
22	B	603	CLA	CMB-C2B-C3B	2.30	131.97	126.55
22	C	503	CLA	C3A-C2A-C1A	2.30	104.79	101.34
24	t	101	BCR	C40-C30-C25	2.30	113.85	110.24
35	V	201	HEC	CHC-C1C-NC	2.30	128.03	123.86
22	B	614	CLA	CHB-C4A-NA	2.30	127.72	124.40
22	D	403	CLA	CED-O2D-CGD	2.30	121.13	115.92
22	A	405	CLA	CMB-C2B-C3B	2.30	131.96	126.55
27	D	408	LMG	O4-C4-C5	2.30	114.98	109.32
22	c	503	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
35	V	201	HEC	CAD-CBD-CGD	-2.30	107.57	113.67
26	D	407	PL9	C50-C49-C48	-2.30	115.76	122.66
30	C	517	DGD	O3D-C3D-C4D	-2.30	104.96	110.38
28	L	102	LHG	C18-C17-C16	-2.30	102.76	114.37
22	C	508	CLA	CHB-C4A-NA	2.30	127.71	124.40
22	a	402	CLA	CHB-C4A-NA	2.30	127.71	124.40
24	k	103	BCR	C2-C1-C6	2.29	113.77	110.44
22	B	606	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
27	A	410	LMG	C9-C8-C7	-2.29	106.44	111.78
24	d	404	BCR	C38-C26-C25	-2.29	121.98	124.48
34	e	101	HEM	CHB-C1B-NB	2.29	127.19	124.37
26	a	410	PL9	C30-C29-C31	2.29	119.19	115.23
22	A	402	CLA	CHC-C1C-NC	2.28	127.75	124.31
28	E	101	LHG	C11-C10-C9	-2.28	102.84	114.37
22	c	508	CLA	O2D-CGD-CBD	2.28	115.22	111.23
22	c	509	CLA	CHB-C4A-NA	2.28	127.69	124.40
22	b	612	CLA	C12-C11-C10	2.28	123.48	113.28
24	A	406	BCR	C8-C7-C6	-2.27	120.92	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	C7-C6-C5	-2.27	107.20	113.26
22	C	506	CLA	C1-C2-C3	-2.27	122.47	126.20
30	c	515	DGD	C4A-C3A-C2A	-2.27	104.77	113.13
22	c	509	CLA	CMB-C2B-C3B	2.27	131.90	126.55
30	C	517	DGD	CDB-CCB-CBB	-2.27	102.88	114.37
22	a	403	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
22	c	504	CLA	CMB-C2B-C3B	2.27	131.89	126.55
23	A	404	PHO	CMA-C3A-C2A	-2.27	105.37	114.13
22	b	606	CLA	O1D-CGD-CBD	2.27	128.99	124.52
22	b	604	CLA	CAA-CBA-CGA	-2.27	106.77	113.21
29	B	622	SQD	C45-O47-C7	2.27	123.22	117.80
27	c	520	LMG	O8-C28-O10	-2.27	117.96	123.63
24	Z	101	BCR	C29-C30-C25	2.26	113.73	110.44
24	D	406	BCR	C7-C8-C9	-2.26	122.89	126.23
22	b	603	CLA	C2D-C1D-ND	-2.26	107.89	110.13
22	B	614	CLA	CHB-C1B-NB	2.26	127.44	124.05
27	a	414	LMG	O6-C1-C2	-2.26	105.72	110.37
22	b	605	CLA	CHD-C1D-ND	-2.26	121.62	124.80
22	c	506	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	A	404	PHO	C3D-C4D-ND	2.26	110.60	107.71
22	b	606	CLA	CHD-C4C-NC	2.26	127.73	124.23
22	B	611	CLA	C5-C3-C2	2.26	126.24	121.17
26	d	405	PL9	C50-C49-C48	-2.26	115.89	122.66
29	f	101	SQD	O5-C5-C4	2.26	113.76	109.70
29	a	412	SQD	C3-C4-C5	2.26	114.32	110.23
34	F	101	HEM	O2D-CGD-CBD	2.25	121.12	114.00
28	d	406	LHG	C18-C17-C16	-2.25	102.98	114.37
22	C	511	CLA	C3B-C4B-NB	-2.25	108.52	110.53
26	d	405	PL9	C40-C39-C38	-2.25	117.84	123.63
29	F	102	SQD	O9-S-O7	-2.25	106.50	113.82
30	c	517	DGD	CAB-C9B-C8B	-2.25	103.00	114.37
22	b	608	CLA	CHD-C1D-ND	-2.25	121.64	124.80
24	B	617	BCR	C15-C16-C17	-2.25	118.92	123.52
30	c	515	DGD	CDB-CCB-CBB	-2.25	103.00	114.37
22	b	610	CLA	CHA-C1A-NA	-2.25	121.30	126.39
24	t	101	BCR	C24-C23-C22	-2.25	122.91	126.23
27	D	411	LMG	C12-C11-C10	-2.25	108.64	114.51
27	A	410	LMG	O6-C1-O1	-2.25	104.73	110.04
29	f	101	SQD	C3-C4-C5	2.25	114.31	110.23
26	d	405	PL9	C8-C7-C3	2.25	117.84	112.03
22	B	604	CLA	C11-C10-C8	-2.24	108.50	115.97
22	B	605	CLA	CAA-CBA-CGA	-2.24	106.84	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	CMB-C2B-C3B	2.24	131.83	126.55
27	A	410	LMG	O5-C6-C5	-2.24	103.69	111.33
35	V	201	HEC	CHC-C4B-C3B	2.24	128.99	125.21
22	c	506	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
22	C	504	CLA	CHA-C1A-NA	-2.24	121.31	126.39
22	a	403	CLA	CHD-C1D-ND	-2.24	121.65	124.80
22	C	509	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
22	B	603	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
30	C	517	DGD	O5E-C6E-C5E	-2.24	103.71	111.33
22	D	405	CLA	CAC-C3C-C4C	2.24	127.70	124.79
22	C	513	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
24	b	618	BCR	C16-C15-C14	-2.24	118.94	123.52
24	B	619	BCR	C15-C16-C17	-2.24	118.94	123.52
24	t	101	BCR	C23-C22-C21	-2.24	115.49	119.01
27	A	410	LMG	C38-C37-C36	-2.24	103.07	114.37
26	D	407	PL9	C36-C34-C33	-2.23	116.15	121.17
34	F	101	HEM	CHB-C1B-NB	2.23	127.13	124.37
22	C	508	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
22	B	616	CLA	C2D-C1D-ND	-2.23	107.92	110.13
22	C	508	CLA	CHD-C1D-ND	-2.23	121.66	124.80
24	b	617	BCR	C11-C10-C9	-2.23	124.15	127.28
22	B	611	CLA	CMB-C2B-C3B	2.23	131.80	126.55
32	t	102	STE	O2-C1-C2	2.23	121.05	114.00
22	C	507	CLA	CAA-CBA-CGA	-2.23	106.88	113.21
22	b	605	CLA	CHB-C1B-NB	2.23	127.39	124.05
22	c	506	CLA	O1D-CGD-CBD	2.23	128.91	124.52
22	b	615	CLA	CAA-CBA-CGA	-2.23	106.89	113.21
22	B	601	CLA	O2D-CGD-CBD	2.23	115.12	111.23
22	C	510	CLA	O2D-CGD-CBD	2.23	115.12	111.23
30	B	623	DGD	C7B-C6B-C5B	-2.23	103.12	114.37
22	C	502	CLA	CHB-C1B-NB	2.23	127.39	124.05
22	C	512	CLA	CMB-C2B-C3B	2.22	131.78	126.55
22	B	615	CLA	C2B-C1B-NB	-2.22	108.02	110.33
34	F	101	HEM	O1D-CGD-CBD	-2.22	116.04	123.09
22	B	608	CLA	CHD-C1D-ND	-2.22	121.67	124.80
22	b	605	CLA	O1A-CGA-CBA	2.22	132.48	123.78
24	c	514	BCR	C36-C18-C19	2.22	121.48	118.09
22	C	507	CLA	CHC-C4B-NB	2.22	127.38	124.05
24	b	619	BCR	C36-C18-C19	2.22	121.48	118.09
30	A	414	DGD	O6D-C1D-O3G	-2.22	104.80	110.04
28	B	621	LHG	C20-C19-C18	-2.22	103.16	114.37
24	k	103	BCR	C8-C7-C6	-2.22	121.07	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C36-C18-C19	2.22	121.47	118.09
30	B	623	DGD	CBB-CAB-C9B	-2.22	103.16	114.37
22	C	502	CLA	O1D-CGD-CBD	2.21	128.89	124.52
27	d	409	LMG	O7-C10-O9	-2.21	118.53	123.70
22	B	604	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
24	H	101	BCR	C16-C15-C14	-2.21	119.00	123.52
22	D	403	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
28	L	102	LHG	C20-C19-C18	-2.21	103.19	114.37
22	c	502	CLA	CHD-C1D-C2D	2.21	130.08	125.49
22	D	405	CLA	CHB-C1B-NB	2.21	127.36	124.05
22	D	403	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
27	D	411	LMG	O9-C10-C11	2.20	130.08	123.09
22	C	510	CLA	CHA-C1A-NA	-2.20	121.40	126.39
22	c	505	CLA	CHD-C4C-NC	2.20	127.65	124.23
29	f	101	SQD	O47-C7-C8	2.20	119.02	110.93
22	c	510	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
24	t	101	BCR	C27-C26-C25	2.20	125.68	122.70
22	d	402	CLA	CHA-C4D-ND	2.20	137.09	132.55
30	c	517	DGD	C3G-C2G-C1G	-2.20	106.65	111.78
22	B	615	CLA	CHA-C4D-ND	2.20	137.09	132.55
22	b	615	CLA	CHC-C1C-NC	2.20	127.62	124.31
24	A	406	BCR	C37-C22-C21	-2.20	119.25	122.82
30	H	102	DGD	O2D-C2D-C1D	-2.20	104.84	110.08
22	C	512	CLA	C2A-C3A-C4A	2.20	105.42	101.87
30	C	517	DGD	C4D-C3D-C2D	-2.20	106.97	110.83
30	h	101	DGD	C4D-C3D-C2D	-2.20	106.97	110.83
22	B	608	CLA	CHB-C4A-NA	2.19	127.57	124.40
26	A	409	PL9	C12-C13-C14	-2.19	122.60	127.62
22	b	602	CLA	C4-C3-C5	2.19	119.03	115.23
22	a	405	CLA	CMD-C2D-C1D	-2.19	120.87	124.73
22	a	403	CLA	C2A-C1A-CHA	2.19	127.67	123.87
22	D	404	CLA	CHD-C1D-ND	-2.19	121.72	124.80
22	B	608	CLA	C1D-ND-C4D	-2.19	104.78	106.31
22	C	510	CLA	CMB-C2B-C3B	2.19	131.69	126.55
28	B	621	LHG	C18-C17-C16	-2.18	103.33	114.37
24	t	101	BCR	C11-C10-C9	-2.18	124.22	127.28
22	b	602	CLA	CHA-C4D-ND	2.18	137.05	132.55
24	K	101	BCR	C36-C18-C19	2.18	121.42	118.09
24	B	619	BCR	C32-C1-C6	-2.18	106.83	110.24
32	B	620	STE	O2-C1-O1	-2.18	117.73	123.33
22	b	610	CLA	CHC-C4B-NB	2.18	127.31	124.05
22	c	510	CLA	C16-C15-C13	-2.17	108.74	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	CHC-C1C-NC	2.17	127.58	124.31
22	b	611	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
32	M	102	STE	O2-C1-O1	-2.17	117.76	123.33
22	C	508	CLA	C7-C6-C5	-2.17	107.49	113.26
22	B	608	CLA	CHC-C4B-NB	2.17	127.30	124.05
24	H	101	BCR	C37-C22-C23	2.17	121.40	118.09
30	B	623	DGD	CAB-C9B-C8B	-2.17	103.42	114.37
22	d	403	CLA	O2D-CGD-O1D	-2.16	119.63	123.85
32	E	102	STE	O2-C1-C2	2.16	120.84	114.00
27	D	408	LMG	C1-C2-C3	-2.16	105.46	110.01
28	E	101	LHG	C18-C17-C16	-2.16	103.44	114.37
30	h	101	DGD	C6D-C5D-C4D	2.16	116.60	112.07
32	a	415	STE	C3-C2-C1	-2.16	108.87	114.51
22	A	403	CLA	C3B-C4B-NB	-2.16	108.60	110.53
22	b	609	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
24	k	103	BCR	C36-C18-C17	-2.16	119.32	122.82
22	C	511	CLA	CAC-C3C-C4C	2.16	127.60	124.79
22	D	403	CLA	CHC-C4B-NB	2.16	127.28	124.05
22	A	402	CLA	CMB-C2B-C3B	2.16	131.62	126.55
29	a	412	SQD	O5-C5-C4	2.16	113.58	109.70
26	D	407	PL9	C30-C29-C31	-2.16	111.49	115.23
22	c	503	CLA	CHC-C4B-NB	2.15	127.28	124.05
22	C	509	CLA	C3B-C4B-NB	-2.15	108.61	110.53
22	B	603	CLA	CHA-C4D-ND	2.15	136.99	132.55
22	b	605	CLA	CHB-C4A-NA	2.15	127.50	124.40
32	C	521	STE	O1-C1-C2	-2.15	116.28	123.09
28	B	621	LHG	C27-C26-C25	-2.15	103.50	114.37
22	B	613	CLA	C3B-C4B-NB	-2.15	108.61	110.53
22	b	613	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
22	c	502	CLA	O1D-CGD-CBD	2.15	128.75	124.52
27	b	622	LMG	C40-C39-C38	-2.15	103.51	114.37
22	A	403	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
22	c	501	CLA	CHD-C1D-ND	-2.15	121.78	124.80
22	b	611	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	C	501	CLA	CHD-C1D-C2D	2.15	129.95	125.49
24	b	619	BCR	C23-C22-C21	2.14	122.38	119.01
22	C	507	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
22	C	508	CLA	CHA-C1A-NA	-2.14	121.54	126.39
22	b	609	CLA	C1-C2-C3	-2.14	122.69	126.20
30	c	516	DGD	C8B-C7B-C6B	-2.14	103.57	114.37
22	B	616	CLA	CMB-C2B-C3B	2.14	131.57	126.55
28	l	101	LHG	C20-C19-C18	-2.14	103.57	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	BCR	C8-C7-C6	-2.13	121.30	127.00
22	B	614	CLA	C1C-C2C-C3C	-2.13	104.74	106.98
28	E	101	LHG	C5-O7-C7	-2.13	112.70	117.80
22	C	509	CLA	C2A-C3A-C4A	2.13	105.31	101.87
22	c	506	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
22	b	608	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
27	c	518	LMG	O6-C1-O1	-2.13	105.02	110.04
22	c	512	CLA	CHD-C1D-C2D	2.13	129.91	125.49
29	B	622	SQD	C3-C4-C5	2.13	114.08	110.23
22	c	507	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
27	M	101	LMG	O1-C7-C8	-2.12	105.66	110.82
22	b	615	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
30	H	102	DGD	O3E-C3E-C2E	-2.12	105.38	110.38
22	D	405	CLA	C1-O2A-CGA	-2.12	111.52	116.65
27	c	518	LMG	C40-C39-C38	-2.12	103.67	114.37
22	C	502	CLA	CMA-C3A-C4A	2.12	117.46	111.77
22	D	405	CLA	C7-C6-C5	-2.12	107.62	113.26
22	B	616	CLA	O1D-CGD-CBD	2.12	128.69	124.52
28	e	102	LHG	C20-C19-C18	-2.12	103.67	114.37
22	C	502	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
22	C	505	CLA	C1-C2-C3	-2.11	122.73	126.20
22	B	605	CLA	C2C-C1C-NC	2.11	112.20	109.98
30	H	102	DGD	CEB-CDB-CCB	-2.11	103.69	114.37
22	b	604	CLA	C4-C3-C5	2.11	118.90	115.23
28	b	623	LHG	C20-C19-C18	-2.11	103.69	114.37
22	c	501	CLA	CHA-C1A-NA	-2.11	121.61	126.39
22	C	502	CLA	CAC-C3C-C4C	2.11	127.54	124.79
23	A	404	PHO	C3D-CAD-CBD	-2.11	104.83	107.61
27	b	622	LMG	O5-C6-C5	-2.11	104.15	111.33
22	d	402	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
22	b	610	CLA	O2D-CGD-CBD	2.11	114.92	111.23
24	K	102	BCR	C15-C16-C17	-2.11	119.21	123.52
24	A	406	BCR	C36-C18-C19	2.11	121.31	118.09
22	b	607	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
22	b	609	CLA	C5-C3-C2	2.10	125.89	121.17
22	B	612	CLA	CHB-C4A-NA	2.10	127.43	124.40
32	J	101	STE	C3-C2-C1	-2.10	109.03	114.51
22	C	513	CLA	C3B-C4B-NB	-2.10	108.66	110.53
22	c	502	CLA	CHB-C4A-NA	2.10	127.43	124.40
22	c	513	CLA	C11-C12-C13	-2.10	108.99	115.97
22	B	603	CLA	CHB-C1B-NB	2.10	127.20	124.05
30	c	517	DGD	C3D-C4D-C5D	-2.10	106.43	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	DGD	C1D-C2D-C3D	-2.10	105.59	110.01
22	b	610	CLA	C1D-ND-C4D	-2.10	104.84	106.31
22	b	612	CLA	C1-C2-C3	-2.10	122.76	126.20
23	a	404	PHO	OBD-CAD-CBD	-2.10	122.75	125.82
22	C	505	CLA	OBD-CAD-C3D	2.10	133.32	128.42
30	C	515	DGD	C6B-C5B-C4B	-2.10	103.77	114.37
24	B	619	BCR	C27-C26-C25	2.10	125.54	122.70
24	K	101	BCR	C12-C13-C14	-2.10	115.71	119.01
22	B	608	CLA	CHD-C4C-NC	2.09	127.48	124.23
27	c	518	LMG	C38-C37-C36	-2.09	103.79	114.37
28	A	411	LHG	O3-P-O5	-2.09	100.64	108.94
22	B	609	CLA	C1C-C2C-C3C	-2.09	104.78	106.98
22	a	405	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
27	M	101	LMG	C1-O6-C5	-2.09	109.64	113.72
23	d	401	PHO	C3D-C4D-ND	2.09	110.39	107.71
22	C	506	CLA	CMB-C2B-C3B	2.09	131.47	126.55
22	C	505	CLA	C11-C10-C8	-2.09	109.02	115.97
22	B	605	CLA	C1-O2A-CGA	-2.09	111.60	116.65
32	C	521	STE	C4-C3-C2	-2.09	105.46	113.13
30	h	101	DGD	CDB-CCB-CBB	-2.09	103.83	114.37
22	C	501	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
22	c	503	CLA	CHB-C4A-NA	2.08	127.41	124.40
22	b	604	CLA	CMA-C3A-C4A	2.08	117.37	111.77
27	A	410	LMG	C1-O6-C5	-2.08	109.66	113.72
22	b	611	CLA	CHD-C1D-C2D	2.08	129.81	125.49
30	C	517	DGD	CAB-C9B-C8B	-2.08	103.85	114.37
27	c	520	LMG	C3-C4-C5	-2.08	106.46	110.23
22	b	602	CLA	CAC-C3C-C4C	2.08	127.50	124.79
34	e	101	HEM	CHD-C4C-NC	2.08	126.72	124.45
22	c	508	CLA	CHB-C1B-NB	2.08	127.17	124.05
30	A	414	DGD	O2E-C2E-C1E	-2.08	105.12	110.08
24	k	102	BCR	C4-C5-C6	2.08	125.51	122.70
22	a	411	CLA	CHC-C1C-NC	2.08	127.44	124.31
22	b	609	CLA	CHA-C1A-NA	-2.08	121.69	126.39
30	h	101	DGD	C1E-O6E-C5E	2.08	117.78	113.72
22	C	511	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	B	613	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	d	403	CLA	CHA-C1A-NA	-2.07	121.70	126.39
22	B	603	CLA	CHD-C1D-ND	-2.07	121.89	124.80
22	c	512	CLA	C4-C3-C5	2.07	118.82	115.23
29	A	412	SQD	O48-C23-O10	-2.07	118.45	123.63
22	A	403	CLA	CHC-C4B-NB	2.07	127.16	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	BCR	C37-C22-C21	-2.07	119.46	122.82
22	b	608	CLA	CHA-C1A-NA	-2.07	121.71	126.39
29	a	412	SQD	O9-S-C6	2.07	109.84	106.76
27	D	408	LMG	C14-C13-C12	-2.06	103.93	114.37
30	c	517	DGD	O3E-C3E-C4E	-2.06	105.51	110.38
24	B	617	BCR	C33-C5-C6	-2.06	122.23	124.48
28	E	101	LHG	C27-C26-C25	-2.06	103.95	114.37
24	B	618	BCR	C2-C1-C6	2.06	113.43	110.44
22	a	403	CLA	CHB-C1B-NB	2.06	127.14	124.05
22	d	403	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
22	B	615	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
28	l	101	LHG	O8-C23-O10	-2.06	118.47	123.63
27	D	408	LMG	C38-C37-C36	-2.06	103.95	114.37
35	v	201	HEC	CMD-C2D-C1D	2.06	128.55	125.42
22	B	610	CLA	CHA-C1A-NA	-2.06	121.73	126.39
26	a	410	PL9	C32-C33-C34	-2.06	122.91	127.62
22	D	405	CLA	CGD-CBD-CAD	-2.06	104.18	110.85
22	C	509	CLA	C6-C7-C8	-2.06	109.13	115.97
24	t	101	BCR	C4-C5-C6	2.06	125.48	122.70
30	c	517	DGD	C3E-C4E-C5E	-2.06	106.50	110.23
22	B	604	CLA	C11-C12-C13	-2.05	109.14	115.97
27	D	410	LMG	O1-C7-C8	-2.05	106.49	111.77
29	F	102	SQD	O8-S-O9	-2.05	106.26	111.40
24	k	101	BCR	C37-C22-C23	2.05	121.22	118.09
22	d	403	CLA	CHD-C1D-ND	-2.05	121.91	124.80
22	C	512	CLA	CHC-C4B-NB	2.05	127.13	124.05
22	B	610	CLA	CAC-C3C-C4C	2.05	127.46	124.79
28	E	101	LHG	C20-C19-C18	-2.05	104.00	114.37
24	D	406	BCR	C30-C25-C26	-2.05	119.83	122.64
22	B	603	CLA	CHA-C1A-NA	-2.05	121.75	126.39
22	B	604	CLA	CGD-CBD-CAD	-2.05	104.22	110.85
22	b	615	CLA	C2B-C1B-NB	-2.05	108.20	110.33
30	c	516	DGD	CBB-CAB-C9B	-2.05	104.02	114.37
22	B	602	CLA	C4-C3-C5	2.05	118.78	115.23
30	h	101	DGD	CBB-CAB-C9B	-2.05	104.03	114.37
22	B	616	CLA	CMB-C2B-C1B	-2.05	122.31	125.42
27	D	410	LMG	C35-C34-C33	-2.04	104.04	114.37
22	C	511	CLA	CHB-C4A-NA	2.04	127.35	124.40
30	H	102	DGD	C4D-C3D-C2D	-2.04	107.25	110.83
22	C	510	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
22	C	504	CLA	CHA-C4D-ND	2.04	136.76	132.55
27	M	101	LMG	C1-C2-C3	-2.04	105.72	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	PHO	CAA-CBA-CGA	-2.04	107.42	113.21
23	A	404	PHO	C4B-NB-C1B	2.04	111.79	108.82
22	B	604	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	B	602	CLA	C3D-C4D-ND	2.04	113.30	109.99
22	b	614	CLA	C4-C3-C5	2.04	118.76	115.23
24	A	406	BCR	C11-C10-C9	-2.04	124.42	127.28
22	B	608	CLA	CMC-C2C-C1C	2.04	128.22	125.03
28	L	102	LHG	C27-C26-C25	-2.04	104.08	114.37
24	k	102	BCR	C8-C7-C6	-2.04	121.56	127.00
22	a	411	CLA	C16-C17-C18	-2.03	106.86	115.94
22	a	405	CLA	CMD-C2D-C3D	2.03	132.35	127.69
22	C	505	CLA	CHB-C1B-NB	2.03	127.10	124.05
32	B	627	STE	C3-C2-C1	-2.03	109.21	114.51
24	b	617	BCR	C36-C18-C17	-2.03	119.53	122.82
22	B	611	CLA	CHD-C4C-NC	2.03	127.38	124.23
30	c	517	DGD	C6B-C5B-C4B	-2.03	104.11	114.37
22	B	601	CLA	O1D-CGD-CBD	2.03	128.52	124.52
22	b	607	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
22	B	607	CLA	CHC-C4B-NB	2.03	127.09	124.05
24	b	619	BCR	C15-C16-C17	-2.03	119.37	123.52
22	b	614	CLA	CHD-C1D-ND	-2.03	121.95	124.80
24	Z	101	BCR	C3-C4-C5	-2.03	110.44	114.06
22	c	512	CLA	CAA-CBA-CGA	-2.03	107.46	113.21
24	k	103	BCR	C15-C16-C17	-2.03	119.38	123.52
30	c	515	DGD	O2G-C1B-O1B	-2.02	118.97	123.70
22	b	602	CLA	CMB-C2B-C3B	2.02	131.31	126.55
22	D	403	CLA	CHD-C4C-NC	2.02	127.37	124.23
22	c	510	CLA	CMB-C2B-C3B	2.02	131.31	126.55
24	A	406	BCR	C38-C26-C27	-2.02	109.29	113.60
22	a	403	CLA	CMB-C2B-C3B	2.02	131.30	126.55
22	B	604	CLA	CHD-C1D-ND	-2.02	121.96	124.80
30	c	515	DGD	C8B-C7B-C6B	-2.02	104.16	114.37
22	d	403	CLA	CHB-C4A-NA	2.02	127.31	124.40
24	H	101	BCR	C1-C6-C5	-2.02	119.88	122.64
29	f	101	SQD	O48-C23-C24	2.02	117.99	111.83
22	D	405	CLA	C6-C7-C8	-2.02	109.26	115.97
22	C	502	CLA	C2D-C1D-ND	-2.02	108.13	110.13
22	b	612	CLA	C14-C13-C15	-2.02	104.08	111.27
24	d	404	BCR	C1-C6-C5	-2.02	119.88	122.64
22	C	504	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
22	D	403	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
30	C	516	DGD	O5D-C1E-C2E	2.01	111.33	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	409	LHG	C18-C17-C16	-2.01	104.18	114.37
22	c	512	CLA	C9-C8-C10	-2.01	104.09	111.27
22	b	611	CLA	CGD-CBD-CAD	-2.01	104.32	110.85
29	L	101	SQD	C1-O5-C5	2.01	117.65	113.72
22	C	502	CLA	C2A-C1A-CHA	2.01	127.36	123.87
22	C	502	CLA	CHA-C1A-NA	-2.01	121.83	126.39
22	c	502	CLA	C1-C2-C3	-2.01	122.90	126.20
22	b	616	CLA	CHD-C1D-ND	-2.01	121.97	124.80
24	K	101	BCR	C8-C7-C6	-2.01	121.63	127.00
30	H	102	DGD	CAB-C9B-C8B	-2.01	104.22	114.37
22	C	502	CLA	C1D-ND-C4D	2.01	107.72	106.31
24	b	618	BCR	C8-C7-C6	-2.01	121.64	127.00
22	C	513	CLA	CMB-C2B-C3B	2.01	131.27	126.55
26	d	405	PL9	C12-C13-C14	-2.01	123.03	127.62
24	B	617	BCR	C8-C7-C6	-2.01	121.64	127.00
27	c	518	LMG	O6-C1-C2	-2.00	106.25	110.37
30	C	517	DGD	O2E-C2E-C3E	-2.00	105.65	110.38
28	b	623	LHG	C27-C26-C25	-2.00	104.24	114.37
22	b	604	CLA	CMC-C2C-C1C	-2.00	121.90	125.03
24	b	618	BCR	C31-C1-C6	2.00	113.38	110.24
24	K	102	BCR	C8-C7-C6	-2.00	121.65	127.00
30	C	517	DGD	C5B-C4B-C3B	-2.00	104.25	114.37
28	D	409	LHG	C27-C26-C25	-2.00	104.25	114.37
22	C	506	CLA	CHB-C4A-NA	2.00	127.29	124.40

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	501	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	D	403	CLA	ND
22	D	404	CLA	ND
22	a	402	CLA	ND
22	a	403	CLA	ND
22	a	405	CLA	ND
22	a	411	CLA	ND
22	b	601	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	c	501	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	d	402	CLA	ND

All (1926) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C6-C7-C8-C9
22	a	403	CLA	C2B-C3B-CAB-CBB
22	a	403	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C11-C10-C8-C9
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	C6-C7-C8-C9
22	b	616	CLA	CHA-CBD-CGD-O2D
22	c	505	CLA	C2B-C3B-CAB-CBB
22	c	505	CLA	C4B-C3B-CAB-CBB
22	c	507	CLA	C4B-C3B-CAB-CBB
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	C11-C12-C13-C14
22	c	512	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C4B-C3B-CAB-CBB
24	A	406	BCR	C20-C21-C22-C37
24	B	617	BCR	C20-C21-C22-C37
24	B	618	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C11-C10-C9-C8
24	B	618	BCR	C10-C11-C12-C13
24	B	619	BCR	C7-C8-C9-C34
24	B	619	BCR	C11-C10-C9-C8
24	C	514	BCR	C11-C12-C13-C14
24	C	514	BCR	C20-C21-C22-C37
24	D	406	BCR	C22-C23-C24-C25
24	H	101	BCR	C35-C13-C14-C15
24	K	101	BCR	C21-C22-C23-C24
24	K	101	BCR	C37-C22-C23-C24
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	T	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C20-C21-C22-C37
24	T	101	BCR	C21-C22-C23-C24
24	Z	101	BCR	C7-C8-C9-C34
24	Z	101	BCR	C14-C15-C16-C17
24	a	406	BCR	C35-C13-C14-C15
24	b	617	BCR	C20-C21-C22-C37
24	b	617	BCR	C21-C22-C23-C24
24	b	619	BCR	C7-C8-C9-C34
24	b	619	BCR	C11-C12-C13-C14
24	b	619	BCR	C16-C17-C18-C36
24	c	514	BCR	C35-C13-C14-C15
24	d	404	BCR	C21-C22-C23-C24
24	d	404	BCR	C37-C22-C23-C24
24	k	101	BCR	C11-C12-C13-C14
24	k	101	BCR	C35-C13-C14-C15
24	k	101	BCR	C13-C14-C15-C16
24	k	101	BCR	C17-C18-C19-C20
24	k	102	BCR	C17-C18-C19-C20
24	k	102	BCR	C36-C18-C19-C20
24	t	101	BCR	C20-C21-C22-C37
24	x	101	BCR	C7-C8-C9-C34
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C37-C38-C39-C41
26	a	410	PL9	C12-C13-C14-C15
26	a	410	PL9	C12-C13-C14-C16
26	a	410	PL9	C17-C18-C19-C20
26	a	410	PL9	C17-C18-C19-C21
26	a	410	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C32-C33-C34-C35
26	a	410	PL9	C37-C38-C39-C40
26	a	410	PL9	C42-C43-C44-C45
26	d	405	PL9	C37-C38-C39-C41
26	d	405	PL9	C42-C43-C44-C45
26	d	405	PL9	C42-C43-C44-C46
27	A	410	LMG	O6-C1-O1-C7
27	A	410	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
27	D	410	LMG	O1-C7-C8-C9
27	D	410	LMG	O1-C7-C8-O7
27	a	414	LMG	O6-C1-O1-C7
27	a	414	LMG	O10-C28-O8-C9
27	a	414	LMG	C29-C28-O8-C9
28	A	411	LHG	C3-O3-P-O5
28	A	411	LHG	C3-O3-P-O6
28	B	621	LHG	C1-C2-C3-O3
28	B	621	LHG	C3-O3-P-O4
28	B	621	LHG	C3-O3-P-O5
28	B	621	LHG	C3-O3-P-O6
28	D	409	LHG	O1-C1-C2-C3
28	D	409	LHG	O2-C2-C3-O3
28	D	409	LHG	C3-O3-P-O4
28	D	409	LHG	C3-O3-P-O5
28	D	409	LHG	C3-O3-P-O6
28	D	409	LHG	C4-O6-P-O4
28	E	101	LHG	C4-O6-P-O4
28	L	102	LHG	C4-O6-P-O3
28	L	102	LHG	C4-O6-P-O4
28	b	623	LHG	O1-C1-C2-O2
28	b	623	LHG	O1-C1-C2-C3
28	b	623	LHG	C1-C2-C3-O3
28	b	623	LHG	C3-O3-P-O5
28	b	623	LHG	C3-O3-P-O6
28	d	406	LHG	O1-C1-C2-C3
28	d	406	LHG	C3-O3-P-O4
28	d	406	LHG	C4-O6-P-O3
28	d	406	LHG	C4-O6-P-O4
28	d	407	LHG	C4-O6-P-O4
28	e	102	LHG	O1-C1-C2-C3
28	e	102	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
28	e	102	LHG	C3-O3-P-O6
28	l	101	LHG	C4-O6-P-O3
28	l	101	LHG	C4-O6-P-O4
28	l	101	LHG	C4-O6-P-O5
29	B	622	SQD	C2-C1-O6-C44
29	B	622	SQD	O5-C1-O6-C44
29	B	622	SQD	O6-C44-C45-O47
29	B	622	SQD	O49-C7-O47-C45
29	B	622	SQD	C8-C7-O47-C45
29	F	102	SQD	C45-C44-O6-C1
29	L	101	SQD	O5-C1-O6-C44
29	L	101	SQD	C8-C7-O47-C45
29	L	101	SQD	O10-C23-O48-C46
29	a	412	SQD	O6-C44-C45-O47
29	a	413	SQD	C8-C7-O47-C45
29	f	101	SQD	O5-C1-O6-C44
30	A	414	DGD	C2B-C1B-O2G-C2G
30	B	623	DGD	C1G-C2G-C3G-O3G
30	B	623	DGD	O2G-C2G-C3G-O3G
35	V	201	HEC	C2B-C3B-CAB-CBB
35	V	201	HEC	C4B-C3B-CAB-CBB
35	V	201	HEC	C2C-C3C-CAC-CBC
35	V	201	HEC	C4C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
35	v	201	HEC	C4B-C3B-CAB-CBB
35	v	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
22	b	601	CLA	O1D-CGD-O2D-CED
22	C	513	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
30	B	623	DGD	O1A-C1A-O1G-C1G
22	b	612	CLA	C8-C10-C11-C12
26	A	409	PL9	C47-C48-C49-C51
26	a	410	PL9	C47-C48-C49-C51
26	d	405	PL9	C47-C48-C49-C50
22	B	601	CLA	CBA-CGA-O2A-C1
27	c	520	LMG	C29-C28-O8-C9
29	L	101	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
22	B	601	CLA	O1A-CGA-O2A-C1
28	e	102	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
29	F	102	SQD	O10-C23-O48-C46
29	f	101	SQD	O10-C23-O48-C46
22	C	513	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	O9-C10-O7-C8
27	b	622	LMG	O9-C10-O7-C8
29	L	101	SQD	O49-C7-O47-C45
29	a	413	SQD	O49-C7-O47-C45
29	f	101	SQD	O49-C7-O47-C45
30	A	414	DGD	O1B-C1B-O2G-C2G
22	B	614	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
28	e	102	LHG	C24-C23-O8-C6
29	F	102	SQD	C24-C23-O48-C46
22	b	614	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	C11-C10-O7-C8
27	D	410	LMG	C11-C10-O7-C8
22	c	509	CLA	O1D-CGD-O2D-CED
27	c	520	LMG	O10-C28-O8-C9
22	A	405	CLA	C4-C3-C5-C6
22	B	605	CLA	C4-C3-C5-C6
22	B	614	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	b	603	CLA	C4-C3-C5-C6
26	A	409	PL9	C35-C34-C36-C37
26	A	409	PL9	C45-C44-C46-C47
26	a	410	PL9	C25-C24-C26-C27
22	C	504	CLA	C2-C3-C5-C6
22	b	603	CLA	C2-C3-C5-C6
26	A	409	PL9	C23-C24-C26-C27
26	a	410	PL9	C18-C19-C21-C22
30	B	623	DGD	C2A-C1A-O1G-C1G
26	D	407	PL9	C32-C33-C34-C35
26	d	405	PL9	C32-C33-C34-C35
26	A	409	PL9	C12-C13-C14-C16
26	D	407	PL9	C32-C33-C34-C36
26	a	410	PL9	C37-C38-C39-C41
26	d	405	PL9	C32-C33-C34-C36
26	A	409	PL9	C47-C48-C49-C50
26	d	405	PL9	C47-C48-C49-C51
22	B	616	CLA	C3-C5-C6-C7
22	c	501	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	A	411	LHG	O2-C2-C3-O3
28	b	623	LHG	O2-C2-C3-O3
22	C	511	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	CBD-CGD-O2D-CED
22	b	605	CLA	C4-C3-C5-C6
26	a	410	PL9	C30-C29-C31-C32
22	A	405	CLA	C2-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
26	A	409	PL9	C43-C44-C46-C47
26	a	410	PL9	C28-C29-C31-C32
26	A	409	PL9	C19-C21-C22-C23
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
26	a	410	PL9	C9-C11-C12-C13
26	a	410	PL9	C14-C16-C17-C18
26	a	410	PL9	C19-C21-C22-C23
26	d	405	PL9	C34-C36-C37-C38
22	D	405	CLA	CBD-CGD-O2D-CED
26	a	410	PL9	C47-C48-C49-C50
27	C	518	LMG	O6-C1-O1-C7
22	C	512	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
24	k	101	BCR	C15-C16-C17-C18
28	D	409	LHG	C1-C2-C3-O3
22	c	506	CLA	CBA-CGA-O2A-C1
27	C	518	LMG	C29-C28-O8-C9
27	M	101	LMG	C29-C28-O8-C9
30	C	517	DGD	C2A-C3A-C4A-C5A
32	b	625	STE	C4-C5-C6-C7
27	A	410	LMG	O6-C5-C6-O5
22	B	613	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	C4-C3-C5-C6
26	A	409	PL9	C40-C39-C41-C42
26	d	405	PL9	C40-C39-C41-C42
22	B	605	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
26	A	409	PL9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
26	D	407	PL9	C38-C39-C41-C42
26	d	405	PL9	C38-C39-C41-C42
22	c	504	CLA	C3-C5-C6-C7
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C6-C7-C8-C9
22	B	601	CLA	C14-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C9
22	B	607	CLA	C14-C13-C15-C16
22	B	614	CLA	C6-C7-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	D	403	CLA	C11-C10-C8-C9
22	D	404	CLA	C14-C13-C15-C16
22	b	603	CLA	C14-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	607	CLA	C14-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C9
22	c	502	CLA	C6-C7-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
22	c	512	CLA	C6-C7-C8-C9
32	b	620	STE	C3-C4-C5-C6
27	C	518	LMG	C2-C1-O1-C7
28	l	101	LHG	C7-C8-C9-C10
28	B	621	LHG	O2-C2-C3-O3
24	B	617	BCR	C36-C18-C19-C20
24	B	619	BCR	C37-C22-C23-C24
24	D	406	BCR	C37-C22-C23-C24
24	K	101	BCR	C7-C8-C9-C34
24	b	619	BCR	C11-C12-C13-C35
24	b	619	BCR	C37-C22-C23-C24
24	k	101	BCR	C11-C12-C13-C35
24	k	102	BCR	C7-C8-C9-C34
24	k	103	BCR	C37-C22-C23-C24
24	t	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C37-C22-C23-C24
28	b	623	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	d	406	LHG	C28-C29-C30-C31
22	c	506	CLA	O1A-CGA-O2A-C1
30	c	517	DGD	O1A-C1A-O1G-C1G
27	A	410	LMG	O1-C7-C8-O7
22	b	603	CLA	C5-C6-C7-C8
22	D	405	CLA	O1D-CGD-O2D-CED
30	H	102	DGD	C2B-C3B-C4B-C5B
22	C	502	CLA	C13-C15-C16-C17
22	C	512	CLA	C10-C11-C12-C13
22	D	405	CLA	C13-C15-C16-C17
22	b	614	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	C13-C15-C16-C17
22	a	403	CLA	C8-C10-C11-C12
22	b	602	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	C2C-C3C-CAC-CBC
22	B	615	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	C	508	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	a	411	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C15
22	B	613	CLA	C13-C15-C16-C17
27	D	410	LMG	C28-C29-C30-C31
26	a	410	PL9	C39-C41-C42-C43
22	B	603	CLA	C8-C10-C11-C12
22	B	606	CLA	C15-C16-C17-C18
22	C	512	CLA	C5-C6-C7-C8
22	b	607	CLA	C8-C10-C11-C12
22	c	508	CLA	C10-C11-C12-C13
30	h	101	DGD	C4E-C5E-C6E-O5E
27	D	411	LMG	C28-C29-C30-C31
27	d	409	LMG	C28-C29-C30-C31
29	L	101	SQD	C7-C8-C9-C10
32	x	102	STE	C1-C2-C3-C4
27	m	101	LMG	C29-C28-O8-C9
22	C	512	CLA	C15-C16-C17-C18
22	b	608	CLA	C8-C10-C11-C12
22	b	612	CLA	C13-C15-C16-C17
22	c	510	CLA	C5-C6-C7-C8
22	c	510	CLA	C8-C10-C11-C12
24	a	406	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C15-C16-C17-C18
22	C	509	CLA	C5-C6-C7-C8
22	a	405	CLA	C5-C6-C7-C8
22	b	601	CLA	C13-C15-C16-C17
22	b	603	CLA	C10-C11-C12-C13
22	c	510	CLA	C10-C11-C12-C13
28	b	623	LHG	C23-C24-C25-C26
28	e	102	LHG	C23-C24-C25-C26
29	L	101	SQD	C23-C24-C25-C26
32	B	627	STE	C1-C2-C3-C4
30	C	516	DGD	O6E-C1E-O5D-C6D
30	C	517	DGD	C4A-C5A-C6A-C7A
22	B	601	CLA	C10-C11-C12-C13
22	B	602	CLA	C13-C15-C16-C17
22	C	503	CLA	C5-C6-C7-C8
22	C	504	CLA	C8-C10-C11-C12
22	C	505	CLA	C10-C11-C12-C13
22	C	509	CLA	C8-C10-C11-C12
22	C	510	CLA	C13-C15-C16-C17
22	C	511	CLA	C8-C10-C11-C12
22	a	402	CLA	C15-C16-C17-C18
22	b	606	CLA	C15-C16-C17-C18
22	b	613	CLA	C10-C11-C12-C13
22	b	614	CLA	C8-C10-C11-C12
22	c	502	CLA	C13-C15-C16-C17
22	c	507	CLA	C13-C15-C16-C17
22	c	511	CLA	C8-C10-C11-C12
28	e	102	LHG	O2-C2-C3-O3
29	F	102	SQD	C44-C45-C46-O48
27	D	408	LMG	C10-C11-C12-C13
27	b	622	LMG	C28-C29-C30-C31
27	m	101	LMG	C10-C11-C12-C13
30	B	623	DGD	C1B-C2B-C3B-C4B
30	c	516	DGD	C1A-C2A-C3A-C4A
32	B	620	STE	C1-C2-C3-C4
22	b	602	CLA	C15-C16-C17-C18
30	A	414	DGD	C4E-C5E-C6E-O5E
22	D	405	CLA	C10-C11-C12-C13
22	c	503	CLA	C5-C6-C7-C8
22	c	502	CLA	CBD-CGD-O2D-CED
27	C	518	LMG	C28-C29-C30-C31
22	b	612	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C5-C6-C7-C8
30	A	414	DGD	C2A-C1A-O1G-C1G
27	b	622	LMG	C11-C10-O7-C8
30	c	516	DGD	C1B-C2B-C3B-C4B
22	C	512	CLA	C3-C5-C6-C7
27	C	518	LMG	O9-C10-O7-C8
28	e	102	LHG	C1-C2-C3-O3
22	B	606	CLA	C2A-CAA-CBA-CGA
29	B	622	SQD	C24-C23-O48-C46
24	k	102	BCR	C14-C15-C16-C17
22	B	601	CLA	C15-C16-C17-C18
22	B	603	CLA	C5-C6-C7-C8
22	B	607	CLA	C5-C6-C7-C8
22	B	609	CLA	C15-C16-C17-C18
22	B	614	CLA	C8-C10-C11-C12
22	B	615	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
22	C	510	CLA	C10-C11-C12-C13
22	C	513	CLA	C15-C16-C17-C18
22	a	411	CLA	C15-C16-C17-C18
22	b	607	CLA	C5-C6-C7-C8
22	b	615	CLA	C15-C16-C17-C18
22	c	511	CLA	C15-C16-C17-C18
22	d	403	CLA	C8-C10-C11-C12
30	C	516	DGD	C1B-C2B-C3B-C4B
22	B	607	CLA	C13-C15-C16-C17
22	B	616	CLA	C5-C6-C7-C8
22	C	507	CLA	C10-C11-C12-C13
22	C	508	CLA	C15-C16-C17-C18
22	b	613	CLA	C15-C16-C17-C18
22	b	614	CLA	C13-C15-C16-C17
22	c	511	CLA	C13-C15-C16-C17
26	A	409	PL9	C38-C39-C41-C42
22	b	612	CLA	C10-C11-C12-C13
22	C	511	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C10-C8-C9
29	f	101	SQD	C2-C1-O6-C44
30	C	516	DGD	C2E-C1E-O5D-C6D
22	a	405	CLA	C10-C11-C12-C13
22	a	405	CLA	CBA-CGA-O2A-C1
24	B	618	BCR	C11-C10-C9-C34
24	C	514	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	D	406	BCR	C20-C21-C22-C37
24	H	101	BCR	C16-C17-C18-C36
24	H	101	BCR	C20-C21-C22-C37
24	K	101	BCR	C11-C10-C9-C34
24	K	101	BCR	C16-C17-C18-C36
24	K	102	BCR	C20-C21-C22-C37
24	a	406	BCR	C11-C10-C9-C34
24	b	618	BCR	C11-C10-C9-C34
24	b	619	BCR	C11-C10-C9-C34
24	b	619	BCR	C20-C21-C22-C37
24	t	101	BCR	C35-C13-C14-C15
22	b	614	CLA	C15-C16-C17-C18
24	c	514	BCR	C36-C18-C19-C20
24	k	102	BCR	C37-C22-C23-C24
24	t	101	BCR	C11-C12-C13-C35
32	B	626	STE	C9-C10-C11-C12
22	b	606	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C5-C6-C7-C8
28	d	407	LHG	O1-C1-C2-C3
29	L	101	SQD	C46-C45-O47-C7
22	C	510	CLA	C16-C17-C18-C20
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
22	b	615	CLA	C3-C5-C6-C7
22	b	607	CLA	C10-C11-C12-C13
22	c	509	CLA	C10-C11-C12-C13
24	B	617	BCR	C12-C13-C14-C15
24	C	514	BCR	C20-C21-C22-C23
24	a	406	BCR	C12-C13-C14-C15
24	b	619	BCR	C12-C13-C14-C15
24	b	619	BCR	C20-C21-C22-C23
24	k	103	BCR	C20-C21-C22-C23
24	t	101	BCR	C11-C10-C9-C8
24	x	101	BCR	C11-C10-C9-C8
22	c	501	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C29-C28-O8-C9
22	b	602	CLA	C13-C15-C16-C17
28	d	407	LHG	C23-C24-C25-C26
22	C	512	CLA	C16-C17-C18-C20
22	a	403	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C16-C17-C18-C20
22	B	607	CLA	C8-C10-C11-C12
27	C	518	LMG	C11-C12-C13-C14
27	D	408	LMG	C37-C38-C39-C40
27	D	411	LMG	C36-C37-C38-C39
28	L	102	LHG	C31-C32-C33-C34
30	C	516	DGD	CCB-CDB-CEB-CFB
30	c	515	DGD	C4B-C5B-C6B-C7B
32	B	626	STE	C12-C13-C14-C15
27	C	518	LMG	C17-C18-C19-C20
27	b	622	LMG	C40-C41-C42-C43
28	A	411	LHG	C30-C31-C32-C33
28	d	406	LHG	C12-C13-C14-C15
29	B	622	SQD	C34-C35-C36-C37
29	F	102	SQD	C27-C28-C29-C30
29	F	102	SQD	C33-C34-C35-C36
29	f	101	SQD	C29-C30-C31-C32
30	A	414	DGD	C9A-CAA-CBA-CCA
30	B	623	DGD	C6A-C7A-C8A-C9A
30	C	516	DGD	C9A-CAA-CBA-CCA
30	c	515	DGD	C4A-C5A-C6A-C7A
32	D	412	STE	C4-C5-C6-C7
32	t	103	STE	C4-C5-C6-C7
23	d	401	PHO	O1D-CGD-O2D-CED
27	b	622	LMG	C11-C12-C13-C14
27	m	101	LMG	C31-C32-C33-C34
28	E	101	LHG	C11-C10-C9-C8
30	C	517	DGD	C8B-C9B-CAB-CBB
30	c	515	DGD	C8B-C9B-CAB-CBB
30	c	515	DGD	CAB-CBB-CCB-CDB
32	E	102	STE	C6-C7-C8-C9
22	C	513	CLA	CBA-CGA-O2A-C1
28	E	101	LHG	C24-C23-O8-C6
30	c	515	DGD	O6D-C5D-C6D-O5D
27	A	410	LMG	C33-C34-C35-C36
27	a	414	LMG	C12-C13-C14-C15
27	a	414	LMG	C31-C32-C33-C34
28	E	101	LHG	C10-C11-C12-C13
28	L	102	LHG	C27-C28-C29-C30
28	b	623	LHG	C33-C34-C35-C36
29	L	101	SQD	C15-C16-C17-C18
29	a	412	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	H	102	DGD	C3B-C4B-C5B-C6B
30	c	516	DGD	C2A-C3A-C4A-C5A
30	c	516	DGD	CCA-CDA-CEA-CFA
32	M	103	STE	C5-C6-C7-C8
32	l	102	STE	C12-C13-C14-C15
28	e	102	LHG	O1-C1-C2-O2
27	A	410	LMG	C29-C30-C31-C32
27	b	622	LMG	C12-C13-C14-C15
27	c	520	LMG	C11-C12-C13-C14
28	A	411	LHG	C12-C13-C14-C15
30	C	515	DGD	C9A-CAA-CBA-CCA
30	C	515	DGD	CAB-CBB-CCB-CDB
30	h	101	DGD	C6B-C7B-C8B-C9B
22	c	503	CLA	C4B-C3B-CAB-CBB
27	D	408	LMG	C15-C16-C17-C18
28	b	623	LHG	C15-C16-C17-C18
30	A	414	DGD	C4B-C5B-C6B-C7B
32	B	625	STE	C9-C10-C11-C12
32	D	412	STE	C11-C10-C9-C8
22	B	605	CLA	C16-C17-C18-C19
22	B	605	CLA	C16-C17-C18-C20
22	a	403	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C14
28	e	102	LHG	C11-C12-C13-C14
30	C	515	DGD	C6A-C7A-C8A-C9A
32	C	519	STE	C4-C5-C6-C7
22	B	606	CLA	C6-C7-C8-C10
22	B	611	CLA	C12-C13-C15-C16
22	B	613	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	b	611	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
27	c	520	LMG	C16-C17-C18-C19
28	D	409	LHG	C14-C15-C16-C17
28	d	406	LHG	C11-C12-C13-C14
29	A	412	SQD	C16-C17-C18-C19
29	F	102	SQD	C28-C29-C30-C31
30	H	102	DGD	C1A-C2A-C3A-C4A
32	E	102	STE	C1-C2-C3-C4
32	J	101	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C12-C13-C14-C15
27	a	414	LMG	C32-C33-C34-C35
27	c	520	LMG	C40-C41-C42-C43
28	L	102	LHG	C17-C18-C19-C20
30	C	516	DGD	C4A-C5A-C6A-C7A
30	c	517	DGD	C5B-C6B-C7B-C8B
32	B	626	STE	C4-C5-C6-C7
32	x	102	STE	C5-C6-C7-C8
22	B	601	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	C32-C33-C34-C35
27	M	101	LMG	C29-C30-C31-C32
27	m	101	LMG	C19-C20-C21-C22
29	f	101	SQD	C32-C33-C34-C35
29	f	101	SQD	C33-C34-C35-C36
27	D	411	LMG	C31-C32-C33-C34
27	M	101	LMG	C14-C15-C16-C17
22	c	510	CLA	C15-C16-C17-C18
28	E	101	LHG	C11-C12-C13-C14
22	C	510	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C19
30	A	414	DGD	O6E-C5E-C6E-O5E
27	c	520	LMG	C30-C31-C32-C33
30	A	414	DGD	CCA-CDA-CEA-CFA
22	B	604	CLA	CBD-CGD-O2D-CED
27	a	414	LMG	C11-C12-C13-C14
27	b	622	LMG	C30-C31-C32-C33
27	m	101	LMG	C30-C31-C32-C33
28	b	623	LHG	C11-C10-C9-C8
29	a	412	SQD	C26-C27-C28-C29
22	C	511	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
28	D	409	LHG	C30-C31-C32-C33
29	A	412	SQD	C9-C10-C11-C12
30	C	517	DGD	C7A-C8A-C9A-CAA
32	I	101	STE	C11-C10-C9-C8
32	l	102	STE	C3-C4-C5-C6
28	E	101	LHG	C23-C24-C25-C26
28	d	406	LHG	C7-C8-C9-C10
30	A	414	DGD	C1A-C2A-C3A-C4A
32	J	101	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	C12-C13-C14-C15
28	L	102	LHG	C14-C15-C16-C17
29	L	101	SQD	C16-C17-C18-C19
30	B	623	DGD	CBA-CCA-CDA-CEA
30	C	515	DGD	CBB-CCB-CDB-CEB
30	h	101	DGD	C3B-C4B-C5B-C6B
32	M	102	STE	C11-C10-C9-C8
32	d	410	STE	C10-C11-C12-C13
27	C	518	LMG	O10-C28-O8-C9
27	c	520	LMG	C39-C40-C41-C42
28	A	411	LHG	C11-C12-C13-C14
29	B	622	SQD	C13-C14-C15-C16
30	A	414	DGD	CBA-CCA-CDA-CEA
32	H	103	STE	C2-C3-C4-C5
32	H	103	STE	C5-C6-C7-C8
32	b	621	STE	C14-C15-C16-C17
32	c	519	STE	C9-C10-C11-C12
28	E	101	LHG	C33-C34-C35-C36
29	A	413	SQD	C32-C33-C34-C35
30	A	414	DGD	CCB-CDB-CEB-CFB
28	A	411	LHG	C25-C26-C27-C28
29	A	413	SQD	C17-C18-C19-C20
30	B	623	DGD	C5A-C6A-C7A-C8A
26	A	409	PL9	C22-C23-C24-C25
22	b	601	CLA	C2B-C3B-CAB-CBB
22	c	507	CLA	C2B-C3B-CAB-CBB
24	D	406	BCR	C23-C24-C25-C26
24	D	406	BCR	C23-C24-C25-C30
24	K	101	BCR	C1-C6-C7-C8
24	K	101	BCR	C5-C6-C7-C8
24	k	102	BCR	C1-C6-C7-C8
24	k	102	BCR	C5-C6-C7-C8
24	t	101	BCR	C1-C6-C7-C8
27	a	414	LMG	C18-C19-C20-C21
30	H	102	DGD	CAB-CBB-CCB-CDB
32	E	102	STE	C4-C5-C6-C7
22	c	508	CLA	CBD-CGD-O2D-CED
29	f	101	SQD	C8-C7-O47-C45
30	B	623	DGD	C2B-C1B-O2G-C2G
27	C	518	LMG	C37-C38-C39-C40
27	D	410	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C38-C39-C40-C41
30	c	515	DGD	C7B-C8B-C9B-CAB
30	c	516	DGD	C4A-C5A-C6A-C7A
32	b	620	STE	C1-C2-C3-C4
22	c	511	CLA	O1D-CGD-O2D-CED
28	d	406	LHG	C14-C15-C16-C17
29	L	101	SQD	C25-C26-C27-C28
30	B	623	DGD	CAB-CBB-CCB-CDB
30	c	517	DGD	C6B-C7B-C8B-C9B
27	d	408	LMG	C36-C37-C38-C39
29	L	101	SQD	C27-C28-C29-C30
29	a	413	SQD	C15-C16-C17-C18
29	a	413	SQD	C17-C18-C19-C20
32	H	103	STE	C7-C8-C9-C10
22	C	511	CLA	O1A-CGA-O2A-C1
22	C	513	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
27	b	622	LMG	C16-C17-C18-C19
28	b	623	LHG	C25-C26-C27-C28
30	A	414	DGD	C9B-CAB-CBB-CCB
32	J	101	STE	C6-C7-C8-C9
32	M	104	STE	C3-C4-C5-C6
27	c	520	LMG	O9-C10-O7-C8
22	c	504	CLA	C4-C3-C5-C6
26	a	410	PL9	C20-C19-C21-C22
22	B	613	CLA	O1D-CGD-O2D-CED
28	B	621	LHG	C28-C29-C30-C31
28	b	623	LHG	C18-C19-C20-C21
32	B	626	STE	C3-C4-C5-C6
32	b	624	STE	C3-C4-C5-C6
24	B	619	BCR	C10-C11-C12-C13
24	C	514	BCR	C18-C19-C20-C21
24	K	102	BCR	C18-C19-C20-C21
24	Z	101	BCR	C10-C11-C12-C13
24	k	101	BCR	C18-C19-C20-C21
22	c	513	CLA	C16-C17-C18-C20
27	d	408	LMG	C31-C32-C33-C34
30	A	414	DGD	C2A-C3A-C4A-C5A
30	B	623	DGD	CEB-CFB-CGB-CHB
27	D	411	LMG	C10-C11-C12-C13
22	B	605	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	c	517	DGD	C2A-C1A-O1G-C1G
22	B	611	CLA	C11-C12-C13-C14
22	b	616	CLA	C6-C7-C8-C9
22	c	511	CLA	C14-C13-C15-C16
27	M	101	LMG	C37-C38-C39-C40
28	d	406	LHG	C29-C30-C31-C32
22	B	612	CLA	C10-C11-C12-C13
27	c	520	LMG	C33-C34-C35-C36
28	D	409	LHG	C34-C35-C36-C37
28	d	407	LHG	C29-C30-C31-C32
32	E	102	STE	C5-C6-C7-C8
32	x	102	STE	C6-C7-C8-C9
24	K	101	BCR	C22-C23-C24-C25
30	c	515	DGD	O6E-C1E-O5D-C6D
30	c	516	DGD	O6E-C1E-O5D-C6D
30	H	102	DGD	C7A-C8A-C9A-CAA
32	m	102	STE	C4-C5-C6-C7
32	x	102	STE	C11-C12-C13-C14
27	a	414	LMG	C2-C1-O1-C7
30	c	516	DGD	C2E-C1E-O5D-C6D
28	l	101	LHG	C14-C15-C16-C17
30	H	102	DGD	C8B-C9B-CAB-CBB
32	J	101	STE	C4-C5-C6-C7
32	c	519	STE	C4-C5-C6-C7
32	c	519	STE	C14-C15-C16-C17
22	C	504	CLA	C11-C12-C13-C14
27	c	520	LMG	C31-C32-C33-C34
29	A	412	SQD	C27-C28-C29-C30
29	A	412	SQD	C29-C30-C31-C32
30	A	414	DGD	C5B-C6B-C7B-C8B
32	B	624	STE	C4-C5-C6-C7
27	A	410	LMG	C31-C32-C33-C34
29	L	101	SQD	C12-C13-C14-C15
22	b	604	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C19
27	c	520	LMG	C11-C10-O7-C8
27	M	101	LMG	C10-C11-C12-C13
28	B	621	LHG	C23-C24-C25-C26
28	A	411	LHG	C24-C25-C26-C27
29	a	412	SQD	C17-C18-C19-C20
30	C	516	DGD	CBB-CCB-CDB-CEB
30	C	515	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C13-C15-C16-C17
24	Z	101	BCR	C11-C12-C13-C35
28	E	101	LHG	C27-C28-C29-C30
30	h	101	DGD	C2B-C3B-C4B-C5B
27	C	518	LMG	C39-C40-C41-C42
29	A	412	SQD	C11-C12-C13-C14
24	B	618	BCR	C11-C12-C13-C14
24	k	102	BCR	C21-C22-C23-C24
27	b	622	LMG	C32-C33-C34-C35
30	c	515	DGD	C6B-C7B-C8B-C9B
22	B	613	CLA	C16-C17-C18-C20
22	b	616	CLA	C11-C12-C13-C15
22	d	402	CLA	C16-C17-C18-C20
28	E	101	LHG	C26-C27-C28-C29
32	B	626	STE	C2-C3-C4-C5
23	A	404	PHO	C4-C3-C5-C6
30	B	623	DGD	C1A-C2A-C3A-C4A
27	a	414	LMG	C33-C34-C35-C36
28	b	623	LHG	C16-C17-C18-C19
30	C	516	DGD	C2B-C3B-C4B-C5B
30	c	517	DGD	C8A-C9A-CAA-CBA
22	c	502	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C16-C17-C18-C19
30	c	515	DGD	C9B-CAB-CBB-CCB
30	c	516	DGD	C8B-C9B-CAB-CBB
30	C	515	DGD	O6E-C5E-C6E-O5E
22	b	611	CLA	C15-C16-C17-C18
22	c	504	CLA	C5-C6-C7-C8
30	c	516	DGD	C5A-C6A-C7A-C8A
32	x	102	STE	C4-C5-C6-C7
30	H	102	DGD	C4B-C5B-C6B-C7B
32	m	102	STE	C5-C6-C7-C8
28	e	102	LHG	O6-C4-C5-O7
30	c	515	DGD	O6E-C5E-C6E-O5E
27	m	101	LMG	C14-C15-C16-C17
28	e	102	LHG	C16-C17-C18-C19
30	h	101	DGD	CAB-CBB-CCB-CDB
32	b	625	STE	C11-C12-C13-C14
34	F	101	HEM	C4C-C3C-CAC-CBC
22	C	511	CLA	C16-C17-C18-C19
27	m	101	LMG	C11-C12-C13-C14
27	m	101	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	C	515	DGD	C4B-C5B-C6B-C7B
32	l	102	STE	C7-C8-C9-C10
22	b	610	CLA	C4C-C3C-CAC-CBC
30	C	516	DGD	C6B-C7B-C8B-C9B
30	C	516	DGD	C8B-C9B-CAB-CBB
30	c	517	DGD	C4B-C5B-C6B-C7B
32	d	410	STE	C5-C6-C7-C8
27	d	409	LMG	O6-C5-C6-O5
29	a	412	SQD	O47-C45-C46-O48
30	A	414	DGD	O2G-C2G-C3G-O3G
27	D	408	LMG	C35-C36-C37-C38
28	d	407	LHG	C33-C34-C35-C36
29	F	102	SQD	C31-C32-C33-C34
30	C	515	DGD	CBA-CCA-CDA-CEA
32	d	410	STE	C9-C10-C11-C12
22	c	512	CLA	O1D-CGD-O2D-CED
30	C	516	DGD	C3A-C4A-C5A-C6A
32	M	104	STE	C10-C11-C12-C13
32	b	621	STE	C2-C3-C4-C5
32	x	102	STE	C10-C11-C12-C13
22	C	512	CLA	C13-C15-C16-C17
28	E	101	LHG	C32-C33-C34-C35
28	d	407	LHG	C32-C33-C34-C35
30	A	414	DGD	C2B-C3B-C4B-C5B
30	c	515	DGD	CBA-CCA-CDA-CEA
30	c	515	DGD	C5B-C6B-C7B-C8B
30	c	515	DGD	C4D-C5D-C6D-O5D
32	b	625	STE	C13-C14-C15-C16
22	b	613	CLA	C16-C17-C18-C19
27	M	101	LMG	C13-C14-C15-C16
28	A	411	LHG	C29-C30-C31-C32
30	H	102	DGD	C5A-C6A-C7A-C8A
30	c	517	DGD	CBB-CCB-CDB-CEB
26	d	405	PL9	C28-C29-C31-C32
27	D	408	LMG	C30-C31-C32-C33
27	M	101	LMG	C20-C21-C22-C23
29	a	412	SQD	C24-C25-C26-C27
30	c	517	DGD	C6A-C7A-C8A-C9A
27	M	101	LMG	C32-C33-C34-C35
27	b	622	LMG	C22-C23-C24-C25
28	L	102	LHG	C12-C13-C14-C15
29	L	101	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	B	625	STE	C12-C13-C14-C15
32	b	620	STE	C2-C3-C4-C5
29	a	413	SQD	C24-C25-C26-C27
32	E	102	STE	C3-C4-C5-C6
22	B	601	CLA	C8-C10-C11-C12
22	B	611	CLA	C8-C10-C11-C12
22	c	508	CLA	C13-C15-C16-C17
27	M	101	LMG	C12-C13-C14-C15
28	B	621	LHG	C25-C26-C27-C28
32	M	102	STE	C7-C8-C9-C10
28	D	409	LHG	C8-C7-O7-C5
32	b	626	STE	C7-C8-C9-C10
27	A	410	LMG	C12-C13-C14-C15
28	B	621	LHG	C29-C30-C31-C32
28	b	623	LHG	C27-C28-C29-C30
28	D	409	LHG	O1-C1-C2-O2
28	d	407	LHG	O1-C1-C2-O2
22	B	605	CLA	O1A-CGA-O2A-C1
22	b	612	CLA	C3-C5-C6-C7
27	d	409	LMG	C11-C12-C13-C14
29	a	412	SQD	C11-C12-C13-C14
29	a	412	SQD	C32-C33-C34-C35
32	H	103	STE	C11-C12-C13-C14
32	b	626	STE	C2-C3-C4-C5
22	c	508	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	502	CLA	C15-C16-C17-C18
29	A	412	SQD	C32-C33-C34-C35
32	l	102	STE	C14-C15-C16-C17
22	B	616	CLA	O1A-CGA-O2A-C1
27	c	520	LMG	C34-C35-C36-C37
27	m	101	LMG	C17-C18-C19-C20
28	e	102	LHG	O6-C4-C5-C6
27	b	622	LMG	C34-C35-C36-C37
30	c	517	DGD	C3A-C4A-C5A-C6A
30	h	101	DGD	CCB-CDB-CEB-CFB
22	C	509	CLA	C3-C5-C6-C7
22	B	601	CLA	C6-C7-C8-C10
22	B	604	CLA	C12-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C10-C8-C7
22	b	607	CLA	C6-C7-C8-C10
22	b	612	CLA	C6-C7-C8-C10
22	b	612	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C12-C13-C15
22	c	508	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C15
22	c	511	CLA	C11-C12-C13-C15
22	d	403	CLA	C6-C7-C8-C10
29	a	413	SQD	C11-C12-C13-C14
30	B	623	DGD	CCA-CDA-CEA-CFA
22	b	605	CLA	C10-C11-C12-C13
22	b	611	CLA	C13-C15-C16-C17
30	c	517	DGD	C2A-C3A-C4A-C5A
22	b	611	CLA	C2-C3-C5-C6
27	c	520	LMG	C36-C37-C38-C39
32	a	415	STE	C6-C7-C8-C9
22	B	606	CLA	C8-C10-C11-C12
22	b	614	CLA	C10-C11-C12-C13
22	B	602	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C12-C13-C14
22	C	511	CLA	C11-C10-C8-C9
22	a	411	CLA	C14-C13-C15-C16
22	b	601	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	b	612	CLA	C6-C7-C8-C9
22	c	502	CLA	C11-C12-C13-C14
22	c	508	CLA	C14-C13-C15-C16
28	D	409	LHG	C29-C30-C31-C32
32	b	621	STE	C5-C6-C7-C8
26	A	409	PL9	C12-C13-C14-C15
27	M	101	LMG	C39-C40-C41-C42
28	b	623	LHG	C29-C30-C31-C32
22	c	507	CLA	O1D-CGD-O2D-CED
27	a	414	LMG	C29-C30-C31-C32
27	m	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
32	t	103	STE	C6-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
27	c	520	LMG	O1-C7-C8-C9
27	m	101	LMG	C7-C8-C9-O8
28	e	102	LHG	C4-C5-C6-O8
29	a	412	SQD	O6-C44-C45-C46
27	A	410	LMG	C4-C5-C6-O5
27	D	410	LMG	C31-C32-C33-C34
27	M	101	LMG	C35-C36-C37-C38
27	D	408	LMG	O6-C5-C6-O5
27	b	622	LMG	O6-C5-C6-O5
27	c	520	LMG	O6-C5-C6-O5
22	c	509	CLA	C16-C17-C18-C19
27	b	622	LMG	C37-C38-C39-C40
30	C	516	DGD	C9B-CAB-CBB-CCB
32	H	103	STE	C9-C10-C11-C12
28	l	101	LHG	C9-C10-C11-C12
29	A	413	SQD	C12-C13-C14-C15
30	C	516	DGD	C5B-C6B-C7B-C8B
24	K	102	BCR	C16-C17-C18-C36
24	Z	101	BCR	C35-C13-C14-C15
24	a	406	BCR	C20-C21-C22-C37
32	x	102	STE	C3-C4-C5-C6
27	D	408	LMG	C39-C40-C41-C42
27	D	410	LMG	C34-C35-C36-C37
23	A	404	PHO	C2-C3-C5-C6
30	C	517	DGD	C4B-C5B-C6B-C7B
30	h	101	DGD	O6E-C5E-C6E-O5E
30	c	515	DGD	O1B-C1B-O2G-C2G
28	d	407	LHG	C34-C35-C36-C37
22	b	604	CLA	C16-C17-C18-C20
22	A	405	CLA	C5-C6-C7-C8
32	D	412	STE	C11-C12-C13-C14
32	a	415	STE	C4-C5-C6-C7
32	b	626	STE	C5-C6-C7-C8
27	c	518	LMG	O6-C5-C6-O5
22	C	513	CLA	C13-C15-C16-C17
22	b	601	CLA	C10-C11-C12-C13
22	b	604	CLA	C15-C16-C17-C18
22	b	611	CLA	C8-C10-C11-C12
22	c	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	CBD-CGD-O2D-CED
27	m	101	LMG	C20-C21-C22-C23
27	m	101	LMG	C37-C38-C39-C40
28	b	623	LHG	C32-C33-C34-C35
32	C	521	STE	C2-C3-C4-C5
28	B	621	LHG	C24-C23-O8-C6
29	a	412	SQD	C24-C23-O48-C46
22	C	512	CLA	O2A-C1-C2-C3
28	l	101	LHG	C15-C16-C17-C18
30	B	623	DGD	C5B-C6B-C7B-C8B
32	B	627	STE	C4-C5-C6-C7
22	B	611	CLA	C13-C15-C16-C17
27	a	414	LMG	C19-C20-C21-C22
27	b	622	LMG	C39-C40-C41-C42
29	A	413	SQD	C15-C16-C17-C18
30	C	515	DGD	C5B-C6B-C7B-C8B
32	I	101	STE	C2-C3-C4-C5
24	T	101	BCR	C13-C14-C15-C16
24	x	101	BCR	C9-C10-C11-C12
28	L	102	LHG	C23-C24-C25-C26
29	a	413	SQD	C29-C30-C31-C32
32	c	519	STE	C15-C16-C17-C18
24	C	514	BCR	C11-C10-C9-C8
24	k	102	BCR	C12-C13-C14-C15
28	L	102	LHG	C10-C11-C12-C13
30	C	516	DGD	C3B-C4B-C5B-C6B
22	B	616	CLA	CBA-CGA-O2A-C1
27	m	101	LMG	C40-C41-C42-C43
27	M	101	LMG	O6-C5-C6-O5
27	D	408	LMG	C36-C37-C38-C39
27	d	408	LMG	C11-C12-C13-C14
30	h	101	DGD	C6A-C7A-C8A-C9A
32	B	625	STE	C4-C5-C6-C7
26	a	410	PL9	C43-C44-C46-C47
27	M	101	LMG	C33-C34-C35-C36
27	b	622	LMG	C31-C32-C33-C34
27	d	408	LMG	C34-C35-C36-C37
22	B	610	CLA	C16-C17-C18-C20
32	H	103	STE	C4-C5-C6-C7
28	A	411	LHG	C23-C24-C25-C26
28	E	101	LHG	C12-C13-C14-C15
30	c	517	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
32	B	627	STE	C5-C6-C7-C8
29	A	412	SQD	O6-C44-C45-O47
32	B	620	STE	C12-C13-C14-C15
28	A	411	LHG	C27-C28-C29-C30
30	B	623	DGD	C6B-C7B-C8B-C9B
32	l	102	STE	C5-C6-C7-C8
27	M	101	LMG	C22-C23-C24-C25
27	A	410	LMG	C36-C37-C38-C39
29	f	101	SQD	C27-C28-C29-C30
32	C	519	STE	C2-C3-C4-C5
32	D	412	STE	C10-C11-C12-C13
32	a	415	STE	C7-C8-C9-C10
29	B	622	SQD	C11-C12-C13-C14
29	a	413	SQD	C14-C15-C16-C17
22	b	606	CLA	C3-C5-C6-C7
32	l	102	STE	C13-C14-C15-C16
30	A	414	DGD	CFA-CGA-CHA-CIA
22	B	614	CLA	C13-C15-C16-C17
26	A	409	PL9	C29-C31-C32-C33
30	B	623	DGD	C4A-C5A-C6A-C7A
28	D	409	LHG	C9-C10-C11-C12
32	C	520	STE	C4-C5-C6-C7
32	b	620	STE	C10-C11-C12-C13
32	b	624	STE	C10-C11-C12-C13
32	d	410	STE	C6-C7-C8-C9
32	l	102	STE	C9-C10-C11-C12
28	L	102	LHG	C19-C20-C21-C22
22	B	616	CLA	CBD-CGD-O2D-CED
27	d	408	LMG	C30-C31-C32-C33
28	L	102	LHG	C18-C19-C20-C21
30	C	516	DGD	C4B-C5B-C6B-C7B
30	c	515	DGD	C2B-C3B-C4B-C5B
22	d	402	CLA	C2C-C3C-CAC-CBC
24	c	514	BCR	C14-C15-C16-C17
27	D	411	LMG	C29-C30-C31-C32
28	d	406	LHG	C15-C16-C17-C18
27	d	408	LMG	C10-C11-C12-C13
30	C	516	DGD	C2A-C3A-C4A-C5A
22	C	512	CLA	C8-C10-C11-C12
22	b	609	CLA	C15-C16-C17-C18
22	D	404	CLA	C16-C17-C18-C20
29	B	622	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C4-C3-C5-C6
26	D	407	PL9	C30-C29-C31-C32
26	a	410	PL9	C45-C44-C46-C47
26	d	405	PL9	C15-C14-C16-C17
32	I	101	STE	C1-C2-C3-C4
28	E	101	LHG	C29-C30-C31-C32
22	D	405	CLA	CBA-CGA-O2A-C1
32	b	620	STE	C13-C14-C15-C16
28	E	101	LHG	C15-C16-C17-C18
28	d	406	LHG	C17-C18-C19-C20
28	d	406	LHG	O1-C1-C2-O2
22	B	604	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	a	411	CLA	C11-C12-C13-C14
22	b	607	CLA	C6-C7-C8-C9
22	b	612	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	D	404	CLA	C15-C16-C17-C18
22	b	615	CLA	C10-C11-C12-C13
27	A	410	LMG	C32-C33-C34-C35
27	C	518	LMG	C30-C31-C32-C33
27	b	622	LMG	C18-C19-C20-C21
28	d	407	LHG	C27-C28-C29-C30
30	c	517	DGD	CCA-CDA-CEA-CFA
32	C	519	STE	C7-C8-C9-C10
32	M	104	STE	C1-C2-C3-C4
22	C	513	CLA	C16-C17-C18-C19
28	D	409	LHG	C15-C16-C17-C18
27	c	520	LMG	C42-C43-C44-C45
27	D	410	LMG	C35-C36-C37-C38
32	H	103	STE	C12-C13-C14-C15
27	d	408	LMG	C35-C36-C37-C38
29	A	412	SQD	C14-C15-C16-C17
22	c	507	CLA	C3-C5-C6-C7
27	b	622	LMG	C24-C25-C26-C27
30	c	516	DGD	CDA-CEA-CFA-CGA
28	E	101	LHG	O6-C4-C5-C6
28	l	101	LHG	O6-C4-C5-C6
28	d	407	LHG	C24-C25-C26-C27
32	c	519	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10
22	C	512	CLA	C6-C7-C8-C10
22	C	512	CLA	C12-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C15
22	a	411	CLA	C11-C12-C13-C15
22	b	601	CLA	C11-C10-C8-C7
22	b	602	CLA	C6-C7-C8-C10
22	b	603	CLA	C11-C10-C8-C7
22	b	605	CLA	C12-C13-C15-C16
22	b	609	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
22	c	513	CLA	C11-C12-C13-C15
30	c	517	DGD	C5A-C6A-C7A-C8A
32	E	102	STE	C7-C8-C9-C10
28	L	102	LHG	C13-C14-C15-C16
28	l	101	LHG	C12-C13-C14-C15
32	l	102	STE	C11-C12-C13-C14
29	L	101	SQD	C30-C31-C32-C33
22	C	505	CLA	C4-C3-C5-C6
22	b	603	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	C2-C3-C5-C6
30	c	515	DGD	C8A-C9A-CAA-CBA
30	h	101	DGD	CBA-CCA-CDA-CEA
30	h	101	DGD	C5B-C6B-C7B-C8B
29	L	101	SQD	C10-C11-C12-C13
29	a	412	SQD	C10-C11-C12-C13
27	M	101	LMG	O10-C28-O8-C9
22	B	607	CLA	C10-C11-C12-C13
27	d	409	LMG	C10-C11-C12-C13
30	C	516	DGD	C6A-C7A-C8A-C9A
27	A	410	LMG	C38-C39-C40-C41
32	c	519	STE	C2-C3-C4-C5
27	a	414	LMG	C17-C18-C19-C20
32	x	102	STE	C9-C10-C11-C12
27	c	520	LMG	C14-C15-C16-C17
32	M	103	STE	C1-C2-C3-C4
27	a	414	LMG	C4-C5-C6-O5
27	M	101	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	d	407	LHG	C35-C36-C37-C38
32	B	620	STE	C7-C8-C9-C10
27	A	410	LMG	O1-C7-C8-C9
29	A	412	SQD	O6-C44-C45-C46
29	B	622	SQD	O6-C44-C45-C46
30	A	414	DGD	O1G-C1G-C2G-C3G
30	A	414	DGD	C1G-C2G-C3G-O3G
30	c	516	DGD	C6A-C7A-C8A-C9A
30	c	516	DGD	C7A-C8A-C9A-CAA
30	c	517	DGD	C1A-C2A-C3A-C4A
22	B	606	CLA	C13-C15-C16-C17
22	D	404	CLA	C13-C15-C16-C17
32	b	624	STE	C2-C3-C4-C5
28	B	621	LHG	C33-C34-C35-C36
28	L	102	LHG	C32-C33-C34-C35
30	B	623	DGD	C7B-C8B-C9B-CAB
30	H	102	DGD	CCA-CDA-CEA-CFA
32	M	104	STE	C11-C10-C9-C8
22	B	615	CLA	C15-C16-C17-C18
22	c	503	CLA	C13-C15-C16-C17
28	l	101	LHG	C17-C18-C19-C20
30	C	517	DGD	C3B-C4B-C5B-C6B
30	h	101	DGD	C3A-C4A-C5A-C6A
22	b	611	CLA	C4-C3-C5-C6
29	a	413	SQD	C11-C10-C9-C8
32	b	624	STE	C9-C10-C11-C12
22	C	510	CLA	C2-C3-C5-C6
22	B	616	CLA	O1D-CGD-O2D-CED
27	b	622	LMG	C13-C14-C15-C16
22	c	508	CLA	C16-C17-C18-C19
28	D	409	LHG	C7-C8-C9-C10
27	D	408	LMG	C12-C13-C14-C15
29	A	412	SQD	C13-C14-C15-C16
24	K	101	BCR	C23-C24-C25-C30
24	b	617	BCR	C1-C6-C7-C8
24	d	404	BCR	C23-C24-C25-C30
24	k	101	BCR	C1-C6-C7-C8
24	t	101	BCR	C5-C6-C7-C8
29	F	102	SQD	C25-C26-C27-C28
32	b	624	STE	C11-C10-C9-C8
32	M	103	STE	C7-C8-C9-C10
27	D	411	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	a	412	SQD	C31-C32-C33-C34
32	D	412	STE	C2-C3-C4-C5
29	a	412	SQD	C30-C31-C32-C33
32	B	620	STE	C6-C7-C8-C9
22	c	513	CLA	C16-C17-C18-C19
27	M	101	LMG	O7-C8-C9-O8
27	c	520	LMG	O1-C7-C8-O7
27	c	520	LMG	O7-C8-C9-O8
28	e	102	LHG	O7-C5-C6-O8
26	a	410	PL9	C4-C3-C7-C8
30	A	414	DGD	CEB-CFB-CGB-CHB
32	B	620	STE	C4-C5-C6-C7
28	b	623	LHG	C13-C14-C15-C16
27	A	410	LMG	C19-C20-C21-C22
30	H	102	DGD	CDB-CEB-CFB-CGB
22	C	506	CLA	C4-C3-C5-C6
26	d	405	PL9	C45-C44-C46-C47
32	t	102	STE	C2-C3-C4-C5
24	k	103	BCR	C10-C11-C12-C13
22	c	509	CLA	CAA-CBA-CGA-O2A
22	C	505	CLA	C2-C3-C5-C6
26	D	407	PL9	C28-C29-C31-C32
28	E	101	LHG	C19-C20-C21-C22
27	a	414	LMG	C16-C17-C18-C19
28	l	101	LHG	C30-C31-C32-C33
29	a	412	SQD	C27-C28-C29-C30
32	D	412	STE	C5-C6-C7-C8
32	x	102	STE	C14-C15-C16-C17
27	A	410	LMG	C14-C15-C16-C17
27	D	411	LMG	C16-C17-C18-C19
29	L	101	SQD	C17-C18-C19-C20
29	L	101	SQD	C29-C30-C31-C32
27	D	410	LMG	C10-C11-C12-C13
27	c	518	LMG	C29-C28-O8-C9
22	B	606	CLA	C11-C12-C13-C14
22	B	616	CLA	C6-C7-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	508	CLA	C14-C13-C15-C16
22	C	512	CLA	C14-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C9
22	c	513	CLA	C11-C12-C13-C14
27	a	414	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	b	619	BCR	C22-C23-C24-C25
24	k	103	BCR	C22-C23-C24-C25
27	d	409	LMG	C34-C35-C36-C37
28	B	621	LHG	C27-C28-C29-C30
24	B	617	BCR	C14-C15-C16-C17
22	B	610	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C19
28	D	409	LHG	C32-C33-C34-C35
30	H	102	DGD	C9A-CAA-CBA-CCA
26	a	410	PL9	C24-C26-C27-C28
28	E	101	LHG	C16-C17-C18-C19
30	B	623	DGD	CBB-CCB-CDB-CEB
30	c	517	DGD	O6D-C5D-C6D-O5D
22	B	615	CLA	C3-C5-C6-C7
24	Z	101	BCR	C15-C16-C17-C18
24	k	102	BCR	C19-C20-C21-C22
28	l	101	LHG	C35-C36-C37-C38
22	C	512	CLA	C16-C17-C18-C19
27	D	408	LMG	C21-C22-C23-C24
32	B	624	STE	C3-C4-C5-C6
28	A	411	LHG	C11-C10-C9-C8
32	c	519	STE	C11-C10-C9-C8
22	A	403	CLA	C8-C10-C11-C12
22	b	610	CLA	C15-C16-C17-C18
24	A	406	BCR	C11-C10-C9-C34
24	A	406	BCR	C16-C17-C18-C36
24	B	618	BCR	C16-C17-C18-C36
24	k	102	BCR	C35-C13-C14-C15
30	A	414	DGD	O1A-C1A-O1G-C1G
22	B	602	CLA	C3-C5-C6-C7
22	C	513	CLA	C8-C10-C11-C12
29	A	412	SQD	C30-C31-C32-C33
30	H	102	DGD	C9B-CAB-CBB-CCB
30	c	515	DGD	C2A-C3A-C4A-C5A
32	B	625	STE	C11-C12-C13-C14
22	B	613	CLA	C16-C17-C18-C19
22	b	610	CLA	C16-C17-C18-C20
32	M	104	STE	C7-C8-C9-C10
22	B	607	CLA	C15-C16-C17-C18
24	k	101	BCR	C7-C8-C9-C34
30	A	414	DGD	C7B-C8B-C9B-CAB
32	d	410	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	C6-C7-C8-C10
22	B	614	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	c	505	CLA	C6-C7-C8-C10
22	c	507	CLA	C6-C7-C8-C10
22	c	512	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C10-C8-C7
32	b	621	STE	C1-C2-C3-C4
28	E	101	LHG	C31-C32-C33-C34
32	b	624	STE	C6-C7-C8-C9
22	B	613	CLA	C15-C16-C17-C18
22	b	603	CLA	C13-C15-C16-C17
24	T	101	BCR	C7-C8-C9-C10
24	b	619	BCR	C21-C22-C23-C24
27	m	101	LMG	C13-C14-C15-C16
22	D	405	CLA	O1A-CGA-O2A-C1
30	C	516	DGD	C2G-C3G-O3G-C1D
30	c	516	DGD	C5D-C6D-O5D-C1E
32	B	626	STE	C6-C7-C8-C9
32	l	102	STE	C4-C5-C6-C7
28	e	102	LHG	C7-C8-C9-C10
22	c	503	CLA	C15-C16-C17-C18
22	b	601	CLA	C2A-CAA-CBA-CGA
22	B	611	CLA	C16-C17-C18-C20
26	A	409	PL9	C12-C11-C9-C10
26	d	405	PL9	C43-C44-C46-C47
30	C	517	DGD	C9B-CAB-CBB-CCB
32	D	412	STE	C9-C10-C11-C12
28	A	411	LHG	C15-C16-C17-C18
22	C	513	CLA	O2A-C1-C2-C3
27	b	622	LMG	C9-C8-O7-C10
29	B	622	SQD	C46-C45-O47-C7
24	b	619	BCR	C9-C10-C11-C12
28	l	101	LHG	C34-C35-C36-C37
30	A	414	DGD	CDA-CEA-CFA-CGA
30	A	414	DGD	CEA-CFA-CGA-CHA
32	b	621	STE	C12-C13-C14-C15
22	C	505	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	H	103	STE	C11-C10-C9-C8
32	B	620	STE	C2-C3-C4-C5
24	T	101	BCR	C20-C21-C22-C23
24	Z	101	BCR	C16-C17-C18-C19
32	t	102	STE	C3-C4-C5-C6
22	c	508	CLA	O1D-CGD-O2D-CED
28	A	411	LHG	O6-C4-C5-O7
28	l	101	LHG	O6-C4-C5-O7
28	A	411	LHG	C10-C11-C12-C13
28	d	406	LHG	C33-C34-C35-C36
29	A	412	SQD	C17-C18-C19-C20
27	c	520	LMG	C7-C8-C9-O8
29	a	412	SQD	C44-C45-C46-O48
29	a	413	SQD	C44-C45-C46-O48
34	e	101	HEM	C4B-C3B-CAB-CBB
22	D	404	CLA	C16-C17-C18-C19
27	A	410	LMG	C35-C36-C37-C38
28	b	623	LHG	C34-C35-C36-C37
27	d	408	LMG	C33-C34-C35-C36
22	B	602	CLA	C8-C10-C11-C12
27	D	408	LMG	C17-C18-C19-C20
28	A	411	LHG	C9-C10-C11-C12
30	A	414	DGD	O1G-C1G-C2G-O2G
30	c	515	DGD	O1G-C1G-C2G-O2G
22	B	605	CLA	C10-C11-C12-C13
22	B	613	CLA	C6-C7-C8-C9
22	C	506	CLA	C11-C12-C13-C14
22	b	606	CLA	C14-C13-C15-C16
22	b	616	CLA	C11-C10-C8-C9
22	c	504	CLA	C6-C7-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	c	507	CLA	C14-C13-C15-C16
22	C	513	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C15
27	D	408	LMG	C14-C15-C16-C17
29	A	413	SQD	C10-C11-C12-C13
27	c	518	LMG	C35-C36-C37-C38
27	c	520	LMG	C15-C16-C17-C18
28	l	101	LHG	C10-C11-C12-C13
29	B	622	SQD	C17-C18-C19-C20
29	L	101	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	CAA-CBA-CCA-CDA
30	C	517	DGD	CBA-CCA-CDA-CEA
32	H	103	STE	C15-C16-C17-C18
29	f	101	SQD	C28-C29-C30-C31
30	c	516	DGD	C5B-C6B-C7B-C8B
29	a	412	SQD	C23-C24-C25-C26
28	L	102	LHG	C29-C30-C31-C32
22	b	602	CLA	C3-C5-C6-C7
30	c	515	DGD	C2E-C1E-O5D-C6D
22	b	601	CLA	CBA-CGA-O2A-C1
22	B	601	CLA	C4-C3-C5-C6
22	b	605	CLA	C15-C16-C17-C18
30	B	623	DGD	C8B-C9B-CAB-CBB
32	B	625	STE	C10-C11-C12-C13
32	l	102	STE	C11-C10-C9-C8
22	b	608	CLA	C16-C17-C18-C19
28	d	407	LHG	C26-C27-C28-C29
32	b	621	STE	C4-C5-C6-C7
22	b	602	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	C4A-C5A-C6A-C7A
29	L	101	SQD	C13-C14-C15-C16
30	H	102	DGD	CCB-CDB-CEB-CFB
22	b	606	CLA	C8-C10-C11-C12
27	A	410	LMG	C40-C41-C42-C43
27	m	101	LMG	C32-C33-C34-C35
22	B	614	CLA	C15-C16-C17-C18
22	c	504	CLA	C8-C10-C11-C12
28	B	621	LHG	C13-C14-C15-C16
22	B	601	CLA	C4B-C3B-CAB-CBB
22	C	504	CLA	C4B-C3B-CAB-CBB
22	C	508	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C1A-C2A-CAA-CBA
22	b	611	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	CBA-CGA-O2A-C1
24	x	101	BCR	C6-C7-C8-C9
32	B	620	STE	C11-C12-C13-C14
28	A	411	LHG	O6-C4-C5-C6
28	b	623	LHG	O9-C7-O7-C5
29	a	412	SQD	C5-C6-S-O9
22	a	403	CLA	C13-C15-C16-C17
22	A	403	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	D	403	CLA	C6-C7-C8-C10
22	a	403	CLA	C12-C13-C15-C16
22	b	604	CLA	C11-C12-C13-C15
22	b	605	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C6-C7-C8-C10
23	a	404	PHO	C6-C7-C8-C10
27	d	409	LMG	C14-C15-C16-C17
28	b	623	LHG	C12-C13-C14-C15
27	D	408	LMG	C38-C39-C40-C41
32	b	625	STE	C6-C7-C8-C9
29	B	622	SQD	C9-C10-C11-C12
32	M	104	STE	C5-C6-C7-C8
30	h	101	DGD	O1A-C1A-O1G-C1G
32	C	520	STE	C2-C3-C4-C5
28	A	411	LHG	C16-C17-C18-C19
32	B	627	STE	C3-C4-C5-C6
27	D	410	LMG	C37-C38-C39-C40
28	d	406	LHG	O9-C7-O7-C5
28	E	101	LHG	O6-C4-C5-O7
30	C	516	DGD	CDB-CEB-CFB-CGB
27	M	101	LMG	C16-C17-C18-C19
22	C	501	CLA	C2A-CAA-CBA-CGA
22	B	615	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	C	501	CLA	O1A-CGA-O2A-C1
27	c	520	LMG	C38-C39-C40-C41
27	M	101	LMG	C15-C16-C17-C18
29	a	413	SQD	C31-C32-C33-C34
32	b	624	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	B	625	STE	C2-C3-C4-C5
30	C	517	DGD	C6B-C7B-C8B-C9B
28	E	101	LHG	O10-C23-O8-C6
27	C	518	LMG	O1-C7-C8-O7
27	b	622	LMG	O1-C7-C8-O7
27	m	101	LMG	O7-C8-C9-O8
27	C	518	LMG	C38-C39-C40-C41
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	611	CLA	C16-C17-C18-C19
30	c	515	DGD	O1G-C1G-C2G-C3G
32	C	520	STE	C11-C12-C13-C14
22	C	506	CLA	C2-C3-C5-C6
32	E	102	STE	C2-C3-C4-C5
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
32	b	620	STE	C5-C6-C7-C8
30	C	515	DGD	O1A-C1A-O1G-C1G
30	C	516	DGD	O6D-C1D-O3G-C3G
29	B	622	SQD	C23-C24-C25-C26
22	C	507	CLA	C16-C17-C18-C20
28	D	409	LHG	C25-C26-C27-C28
27	M	101	LMG	C34-C35-C36-C37
22	c	509	CLA	C13-C15-C16-C17
30	A	414	DGD	CBB-CCB-CDB-CEB
32	c	519	STE	C7-C8-C9-C10
28	L	102	LHG	O10-C23-O8-C6
22	A	405	CLA	C6-C7-C8-C9
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	513	CLA	CAD-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	H	101	BCR	C9-C10-C11-C12
24	T	101	BCR	C9-C10-C11-C12
24	Z	101	BCR	C13-C14-C15-C16
24	k	101	BCR	C9-C10-C11-C12
28	E	101	LHG	C4-O6-P-O3
28	d	407	LHG	C4-O6-P-O3
28	e	102	LHG	C3-O3-P-O4
29	A	413	SQD	C46-C45-O47-C7
30	c	517	DGD	CCB-CDB-CEB-CFB
22	c	510	CLA	C16-C17-C18-C19
27	b	622	LMG	C17-C18-C19-C20
22	c	503	CLA	C2B-C3B-CAB-CBB
29	a	413	SQD	C26-C27-C28-C29
22	B	601	CLA	C2-C3-C5-C6
28	E	101	LHG	C18-C19-C20-C21
24	K	101	BCR	C11-C12-C13-C35
24	b	617	BCR	C7-C8-C9-C34
28	d	407	LHG	C2-C3-O3-P
28	b	623	LHG	C28-C29-C30-C31
22	B	605	CLA	C8-C10-C11-C12
32	I	101	STE	C5-C6-C7-C8
27	c	520	LMG	C41-C42-C43-C44
30	B	623	DGD	CDA-CEA-CFA-CGA
22	B	605	CLA	C3-C5-C6-C7
27	A	410	LMG	C28-C29-C30-C31
28	D	409	LHG	C33-C34-C35-C36
29	a	413	SQD	C16-C17-C18-C19
22	b	608	CLA	C2C-C3C-CAC-CBC
27	a	414	LMG	C36-C37-C38-C39
22	C	507	CLA	C16-C17-C18-C19
30	c	517	DGD	CDA-CEA-CFA-CGA
32	M	104	STE	C2-C3-C4-C5
27	D	410	LMG	C9-C8-O7-C10
30	B	623	DGD	C3G-C2G-O2G-C1B
27	A	410	LMG	C39-C40-C41-C42
32	C	519	STE	C5-C6-C7-C8
30	C	515	DGD	O6D-C5D-C6D-O5D
22	B	601	CLA	C13-C15-C16-C17
22	B	613	CLA	C5-C6-C7-C8
22	a	411	CLA	C8-C10-C11-C12
32	B	624	STE	C7-C8-C9-C10
32	t	103	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C16-C17-C18-C20
28	B	621	LHG	C24-C25-C26-C27
22	c	502	CLA	C3-C5-C6-C7
22	b	609	CLA	C13-C15-C16-C17
22	B	603	CLA	C11-C10-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C12-C13-C14
22	b	612	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C10-C8-C9
22	B	606	CLA	C12-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C10-C8-C7
24	B	617	BCR	C20-C21-C22-C23
24	B	619	BCR	C20-C21-C22-C23
24	H	101	BCR	C20-C21-C22-C23
24	Z	101	BCR	C11-C10-C9-C8
28	A	411	LHG	C1-C2-C3-O3
32	m	102	STE	C3-C4-C5-C6
24	B	619	BCR	C22-C23-C24-C25
30	c	516	DGD	C8A-C9A-CAA-CBA
28	d	406	LHG	C31-C32-C33-C34
30	C	515	DGD	C4D-C5D-C6D-O5D
30	H	102	DGD	C8A-C9A-CAA-CBA
27	m	101	LMG	C12-C13-C14-C15
30	h	101	DGD	C2A-C3A-C4A-C5A
30	C	515	DGD	C3B-C4B-C5B-C6B
22	B	603	CLA	C10-C11-C12-C13
28	b	623	LHG	C14-C15-C16-C17
29	F	102	SQD	C30-C31-C32-C33
32	b	626	STE	C3-C4-C5-C6
30	c	516	DGD	C9A-CAA-CBA-CCA
22	B	608	CLA	C5-C6-C7-C8
28	l	101	LHG	C28-C29-C30-C31
32	B	627	STE	C6-C7-C8-C9
22	C	506	CLA	C15-C16-C17-C18
28	L	102	LHG	C30-C31-C32-C33
28	e	102	LHG	C25-C26-C27-C28
28	e	102	LHG	C27-C28-C29-C30
29	L	101	SQD	C26-C27-C28-C29
29	a	413	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	c	516	DGD	C7B-C8B-C9B-CAB
28	A	411	LHG	C31-C32-C33-C34
22	b	610	CLA	C16-C17-C18-C19
30	h	101	DGD	O2G-C1B-C2B-C3B
27	b	622	LMG	O1-C7-C8-C9
30	H	102	DGD	O2G-C1B-C2B-C3B
22	d	403	CLA	C16-C17-C18-C19
28	B	621	LHG	C16-C17-C18-C19
30	c	516	DGD	C2G-C3G-O3G-C1D
27	D	410	LMG	C29-C30-C31-C32
30	H	102	DGD	C5B-C6B-C7B-C8B
32	d	410	STE	C2-C3-C4-C5
22	B	603	CLA	C2A-CAA-CBA-CGA
22	c	509	CLA	C2A-CAA-CBA-CGA
24	k	103	BCR	C19-C20-C21-C22
28	L	102	LHG	C24-C25-C26-C27
22	c	510	CLA	O1D-CGD-O2D-CED
27	d	409	LMG	C15-C16-C17-C18
28	e	102	LHG	C18-C19-C20-C21
32	t	102	STE	C6-C7-C8-C9
27	d	409	LMG	C37-C38-C39-C40
30	c	517	DGD	C7B-C8B-C9B-CAB
22	a	411	CLA	C16-C17-C18-C19
30	C	515	DGD	O1G-C1A-C2A-C3A
22	C	506	CLA	C6-C7-C8-C9
22	a	403	CLA	C6-C7-C8-C9
22	a	403	CLA	C14-C13-C15-C16
22	b	602	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C12-C13-C14
22	b	611	CLA	C14-C13-C15-C16
22	A	405	CLA	CBA-CGA-O2A-C1
28	A	411	LHG	C2-C3-O3-P
27	D	410	LMG	C30-C31-C32-C33
32	l	102	STE	C6-C7-C8-C9
32	l	102	STE	C10-C11-C12-C13
27	D	411	LMG	C32-C33-C34-C35
28	L	102	LHG	C11-C12-C13-C14
22	d	402	CLA	C13-C15-C16-C17
27	b	622	LMG	C23-C24-C25-C26
32	C	519	STE	O2-C1-C2-C3
28	d	406	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	b	625	STE	C7-C8-C9-C10
32	c	519	STE	C11-C12-C13-C14
22	C	513	CLA	C12-C13-C15-C16
22	a	403	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C12-C13-C15
22	A	405	CLA	O1A-CGA-O2A-C1
28	b	623	LHG	C10-C11-C12-C13
32	I	101	STE	C7-C8-C9-C10
32	m	102	STE	C6-C7-C8-C9
27	C	518	LMG	C33-C34-C35-C36
27	d	408	LMG	C38-C39-C40-C41
29	B	622	SQD	C24-C25-C26-C27
29	L	101	SQD	C24-C25-C26-C27
24	T	101	BCR	C11-C10-C9-C34
24	Z	101	BCR	C20-C21-C22-C37
24	c	514	BCR	C20-C21-C22-C37
22	B	610	CLA	C15-C16-C17-C18
35	v	201	HEC	CAD-CBD-CGD-O1D
35	v	201	HEC	CAD-CBD-CGD-O2D
22	b	612	CLA	C2C-C3C-CAC-CBC
27	c	520	LMG	C37-C38-C39-C40
22	a	411	CLA	C13-C15-C16-C17
22	c	508	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
22	B	603	CLA	C16-C17-C18-C19
27	d	409	LMG	C32-C33-C34-C35
32	B	624	STE	O1-C1-C2-C3
35	V	201	HEC	CAD-CBD-CGD-O1D
32	I	101	STE	C3-C4-C5-C6
22	c	513	CLA	C3-C5-C6-C7
32	D	412	STE	O1-C1-C2-C3
22	B	614	CLA	C11-C12-C13-C14
22	b	603	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
29	A	413	SQD	C27-C28-C29-C30
27	D	411	LMG	O9-C10-C11-C12
27	D	411	LMG	O10-C28-C29-C30
32	C	519	STE	O1-C1-C2-C3
22	A	402	CLA	C15-C16-C17-C18
32	B	624	STE	O2-C1-C2-C3
35	V	201	HEC	CAD-CBD-CGD-O2D
27	c	518	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
32	b	620	STE	C7-C8-C9-C10
28	A	411	LHG	C35-C36-C37-C38
29	a	412	SQD	C19-C20-C21-C22
22	B	604	CLA	C10-C11-C12-C13
22	B	614	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	D	405	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C16-C17-C18-C19
23	a	404	PHO	C5-C6-C7-C8
27	m	101	LMG	O6-C1-O1-C7
22	C	512	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	C8-C10-C11-C12
22	B	601	CLA	C2B-C3B-CAB-CBB
22	C	504	CLA	C2B-C3B-CAB-CBB
22	b	607	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C1-C6-C7-C8
24	b	617	BCR	C5-C6-C7-C8
24	d	404	BCR	C23-C24-C25-C26
24	k	101	BCR	C5-C6-C7-C8
24	k	101	BCR	C23-C24-C25-C30
24	k	103	BCR	C23-C24-C25-C30
22	b	608	CLA	C4C-C3C-CAC-CBC
32	D	412	STE	O2-C1-C2-C3
22	C	512	CLA	CBA-CGA-O2A-C1
30	c	515	DGD	C5A-C6A-C7A-C8A
30	c	516	DGD	C3A-C4A-C5A-C6A
27	c	518	LMG	C31-C32-C33-C34
32	D	412	STE	C14-C15-C16-C17
22	c	511	CLA	C16-C17-C18-C20
27	D	408	LMG	C33-C34-C35-C36
32	c	519	STE	O2-C1-C2-C3
30	h	101	DGD	C5A-C6A-C7A-C8A
27	c	520	LMG	C28-C29-C30-C31
27	D	408	LMG	C11-C12-C13-C14
32	B	625	STE	O2-C1-C2-C3
22	B	602	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C12-C13-C15
22	B	613	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	D	405	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	b	602	CLA	C12-C13-C15-C16
22	b	612	CLA	C11-C10-C8-C7
22	b	615	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
29	A	413	SQD	C29-C30-C31-C32
32	B	625	STE	C5-C6-C7-C8
22	c	505	CLA	C16-C17-C18-C20
27	D	411	LMG	O8-C28-C29-C30
32	c	519	STE	O1-C1-C2-C3
29	A	413	SQD	C25-C26-C27-C28
27	M	101	LMG	C19-C20-C21-C22
23	D	401	PHO	C2C-C3C-CAC-CBC
26	A	409	PL9	C4-C3-C7-C8
28	l	101	LHG	C13-C14-C15-C16
29	F	102	SQD	C34-C35-C36-C37
30	C	517	DGD	C6A-C7A-C8A-C9A
27	d	409	LMG	C40-C41-C42-C43
32	x	102	STE	O1-C1-C2-C3
29	A	412	SQD	C7-C8-C9-C10
22	C	512	CLA	C4-C3-C5-C6
22	b	615	CLA	C8-C10-C11-C12
22	c	508	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	B	604	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	CDA-CEA-CFA-CGA
22	c	509	CLA	C8-C10-C11-C12
32	B	625	STE	O1-C1-C2-C3
32	j	101	STE	C3-C4-C5-C6
32	b	621	STE	O2-C1-C2-C3
22	B	607	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C12-C13-C14
32	t	103	STE	C5-C6-C7-C8
24	K	102	BCR	C9-C10-C11-C12
29	L	101	SQD	C28-C29-C30-C31
32	B	625	STE	C6-C7-C8-C9
29	A	413	SQD	C11-C10-C9-C8
32	l	102	STE	C15-C16-C17-C18
27	c	518	LMG	C40-C41-C42-C43
22	C	513	CLA	C4-C3-C5-C6
22	a	405	CLA	C4-C3-C5-C6
30	c	517	DGD	C9B-CAB-CBB-CCB
22	a	405	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	d	405	PL9	C18-C19-C21-C22
27	D	411	LMG	C34-C35-C36-C37
22	b	603	CLA	C15-C16-C17-C18
22	B	612	CLA	CBA-CGA-O2A-C1
32	b	621	STE	O1-C1-C2-C3
22	c	512	CLA	C15-C16-C17-C18
22	d	402	CLA	C15-C16-C17-C18
30	h	101	DGD	C7A-C8A-C9A-CAA
30	C	515	DGD	CDA-CEA-CFA-CGA
26	A	409	PL9	C39-C41-C42-C43
27	D	410	LMG	C7-C8-C9-O8
30	C	515	DGD	O1G-C1G-C2G-C3G
27	D	411	LMG	O7-C10-C11-C12
32	x	102	STE	O2-C1-C2-C3
22	b	610	CLA	C2A-CAA-CBA-CGA
27	D	411	LMG	C35-C36-C37-C38
32	M	102	STE	C9-C10-C11-C12
22	b	605	CLA	C5-C6-C7-C8
28	e	102	LHG	C14-C15-C16-C17
23	a	404	PHO	C4-C3-C5-C6
27	c	518	LMG	C33-C34-C35-C36
22	a	405	CLA	C15-C16-C17-C18
22	C	507	CLA	C4B-C3B-CAB-CBB
32	M	104	STE	C12-C13-C14-C15
23	a	404	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O1D
22	D	403	CLA	C3-C5-C6-C7
28	d	406	LHG	C9-C10-C11-C12
29	L	101	SQD	O6-C44-C45-O47
29	L	101	SQD	O47-C45-C46-O48
22	c	502	CLA	C2C-C3C-CAC-CBC
29	A	413	SQD	C7-C8-C9-C10
22	C	513	CLA	C2-C3-C5-C6
28	e	102	LHG	C2-C3-O3-P
32	B	624	STE	C5-C6-C7-C8
22	C	507	CLA	C6-C7-C8-C10
22	c	509	CLA	C6-C7-C8-C10
28	d	406	LHG	C30-C31-C32-C33
28	L	102	LHG	C9-C10-C11-C12
30	C	515	DGD	C6B-C7B-C8B-C9B
32	I	101	STE	C10-C11-C12-C13
22	C	504	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C11-C12-C13-C14
23	a	404	PHO	C6-C7-C8-C9
30	B	623	DGD	C2B-C3B-C4B-C5B
27	c	520	LMG	C29-C30-C31-C32
32	d	410	STE	C3-C4-C5-C6
27	M	101	LMG	C8-C7-O1-C1
29	a	412	SQD	C5-C6-S-O8
22	B	613	CLA	C2-C1-O2A-CGA
22	d	402	CLA	C2-C1-O2A-CGA
22	B	612	CLA	O1A-CGA-O2A-C1
26	a	410	PL9	C21-C22-C23-C24
22	c	502	CLA	C4C-C3C-CAC-CBC
22	B	603	CLA	C16-C17-C18-C20
22	C	508	CLA	C5-C6-C7-C8
22	B	604	CLA	CBA-CGA-O2A-C1
23	d	401	PHO	C3A-C2A-CAA-CBA
22	c	509	CLA	CAA-CBA-CGA-O1A
30	c	515	DGD	O1G-C1A-C2A-C3A
27	a	414	LMG	C39-C40-C41-C42
27	D	408	LMG	C13-C14-C15-C16
27	D	408	LMG	C16-C17-C18-C19
27	D	410	LMG	C16-C17-C18-C19
32	j	101	STE	C7-C8-C9-C10
27	M	101	LMG	C28-C29-C30-C31
27	b	622	LMG	C10-C11-C12-C13
27	A	410	LMG	C7-C8-O7-C10
30	B	623	DGD	C1G-C2G-O2G-C1B
24	b	619	BCR	C14-C15-C16-C17
22	b	608	CLA	C16-C17-C18-C20
23	d	401	PHO	C8-C10-C11-C12
29	f	101	SQD	C26-C27-C28-C29
30	c	516	DGD	CCB-CDB-CEB-CFB
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
24	b	619	BCR	C16-C17-C18-C19
24	t	101	BCR	C20-C21-C22-C23
27	d	409	LMG	C35-C36-C37-C38
22	B	606	CLA	C10-C11-C12-C13
23	A	404	PHO	CBA-CGA-O2A-C1
26	A	409	PL9	C9-C11-C12-C13
22	C	513	CLA	C3-C5-C6-C7
29	A	412	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	D	407	PL9	C45-C44-C46-C47
22	b	612	CLA	CAA-CBA-CGA-O2A
22	b	601	CLA	C16-C17-C18-C19
27	m	101	LMG	C29-C30-C31-C32
30	C	515	DGD	C8B-C9B-CAB-CBB
32	k	104	STE	O2-C1-C2-C3
29	a	412	SQD	O47-C7-C8-C9
22	c	505	CLA	C5-C6-C7-C8
32	x	102	STE	C11-C10-C9-C8
27	a	414	LMG	O6-C5-C6-O5
22	a	405	CLA	C6-C7-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C12-C13-C14
28	d	406	LHG	C16-C17-C18-C19
22	C	502	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	C10-C11-C12-C13
32	b	626	STE	C4-C5-C6-C7
24	d	404	BCR	C7-C8-C9-C10
32	J	101	STE	C2-C3-C4-C5
22	B	609	CLA	C4-C3-C5-C6
22	C	502	CLA	O1A-CGA-O2A-C1
27	c	518	LMG	C30-C31-C32-C33
28	E	101	LHG	O8-C23-C24-C25
22	c	502	CLA	C16-C17-C18-C19
22	B	602	CLA	C11-C10-C8-C7
22	B	603	CLA	C6-C7-C8-C10
22	D	403	CLA	C12-C13-C15-C16
22	a	405	CLA	C12-C13-C15-C16
22	b	603	CLA	C6-C7-C8-C10
22	b	603	CLA	C12-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C10
22	b	614	CLA	C12-C13-C15-C16
22	c	511	CLA	C12-C13-C15-C16
22	c	512	CLA	C11-C12-C13-C15
32	k	104	STE	O1-C1-C2-C3
22	B	609	CLA	C2B-C3B-CAB-CBB
22	b	612	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
24	k	101	BCR	C23-C24-C25-C26
24	k	102	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	k	103	BCR	C1-C6-C7-C8
24	k	103	BCR	C23-C24-C25-C26
29	a	412	SQD	C8-C7-O47-C45
30	C	516	DGD	O1B-C1B-O2G-C2G
22	A	402	CLA	C2-C1-O2A-CGA
22	C	512	CLA	C2-C1-O2A-CGA
27	a	414	LMG	C35-C36-C37-C38
30	H	102	DGD	C6A-C7A-C8A-C9A
22	c	508	CLA	C15-C16-C17-C18
30	B	623	DGD	CFA-CGA-CHA-CIA
27	m	101	LMG	O8-C28-C29-C30
29	a	413	SQD	O48-C23-C24-C25
22	B	612	CLA	CAA-CBA-CGA-O2A
23	a	404	PHO	C2-C3-C5-C6
22	B	601	CLA	C2A-CAA-CBA-CGA
28	e	102	LHG	C8-C7-O7-C5
29	A	412	SQD	O47-C7-C8-C9
27	m	101	LMG	C35-C36-C37-C38
22	a	411	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C20
28	E	101	LHG	C17-C18-C19-C20
30	C	516	DGD	C5A-C6A-C7A-C8A
28	L	102	LHG	C7-C8-C9-C10
22	b	614	CLA	O1A-CGA-O2A-C1
22	c	502	CLA	C16-C17-C18-C20
34	F	101	HEM	CAD-CBD-CGD-O1D
29	A	413	SQD	C28-C29-C30-C31
22	a	411	CLA	C4C-C3C-CAC-CBC
32	H	103	STE	C1-C2-C3-C4
22	A	403	CLA	C11-C12-C13-C14
22	D	403	CLA	C6-C7-C8-C9
22	D	405	CLA	C6-C7-C8-C9
24	D	406	BCR	C7-C8-C9-C34
22	a	411	CLA	C1A-C2A-CAA-CBA
22	a	411	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C1A-C2A-CAA-CBA
32	b	621	STE	C11-C10-C9-C8
26	A	409	PL9	C21-C22-C23-C24
27	a	414	LMG	C15-C16-C17-C18
24	H	101	BCR	C17-C18-C19-C20
30	c	515	DGD	C7A-C8A-C9A-CAA
22	c	507	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C2A-CAA-CBA-CGA
28	l	101	LHG	O7-C7-C8-C9
30	C	515	DGD	O2G-C1B-C2B-C3B
29	a	412	SQD	C5-C6-S-O7
22	c	505	CLA	C15-C16-C17-C18
22	B	601	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C2-C1-O2A-CGA
22	b	610	CLA	C2-C1-O2A-CGA
22	B	604	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C12-C13-C15
22	C	509	CLA	C11-C12-C13-C15
22	C	511	CLA	C12-C13-C15-C16
22	D	403	CLA	C11-C10-C8-C7
22	c	502	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C12-C13-C15
30	C	517	DGD	O6D-C5D-C6D-O5D
22	B	613	CLA	CAA-CBA-CGA-O2A
30	C	516	DGD	CAA-CBA-CCA-CDA
26	d	405	PL9	C11-C12-C13-C14
26	d	405	PL9	C44-C46-C47-C48
22	b	614	CLA	C16-C17-C18-C20
24	T	101	BCR	C12-C13-C14-C15
34	F	101	HEM	CAD-CBD-CGD-O2D
28	E	101	LHG	C34-C35-C36-C37
29	A	413	SQD	C18-C19-C20-C21
22	C	511	CLA	C15-C16-C17-C18
27	d	409	LMG	C30-C31-C32-C33
28	e	102	LHG	C10-C11-C12-C13
26	d	405	PL9	C46-C47-C48-C49
30	c	515	DGD	O1B-C1B-C2B-C3B
22	d	402	CLA	C3-C5-C6-C7
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	b	614	CLA	C14-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C9
30	A	414	DGD	C6A-C7A-C8A-C9A
32	B	620	STE	C9-C10-C11-C12
24	x	101	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C17-C18-C19-C20
27	M	101	LMG	O10-C28-C29-C30
29	A	412	SQD	O49-C7-C8-C9
32	c	519	STE	C10-C11-C12-C13
32	M	102	STE	O2-C1-C2-C3
24	x	101	BCR	C7-C8-C9-C10
29	a	413	SQD	C24-C23-O48-C46
22	B	612	CLA	CAA-CBA-CGA-O1A
30	C	515	DGD	C5D-C6D-O5D-C1E
30	H	102	DGD	C2G-C3G-O3G-C1D
22	B	613	CLA	CAA-CBA-CGA-O1A
30	C	515	DGD	O1B-C1B-C2B-C3B
27	C	518	LMG	O7-C10-C11-C12
22	B	610	CLA	C2A-CAA-CBA-CGA
27	M	101	LMG	O1-C7-C8-C9
29	L	101	SQD	C44-C45-C46-O48
30	c	515	DGD	C1G-C2G-C3G-O3G
32	B	627	STE	O2-C1-C2-C3
22	b	616	CLA	C4C-C3C-CAC-CBC
22	b	612	CLA	CAA-CBA-CGA-O1A
22	B	608	CLA	C4-C3-C5-C6
22	b	616	CLA	C10-C11-C12-C13
22	d	403	CLA	C10-C11-C12-C13
30	c	516	DGD	C4E-C5E-C6E-O5E
32	b	624	STE	C11-C12-C13-C14
22	B	609	CLA	CAD-CBD-CGD-O2D
22	B	612	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	C2C-C3C-CAC-CBC
27	D	411	LMG	C11-C12-C13-C14
27	A	410	LMG	C37-C38-C39-C40
30	C	516	DGD	O1B-C1B-C2B-C3B
32	C	520	STE	C5-C6-C7-C8
22	b	613	CLA	CAA-CBA-CGA-O2A
28	e	102	LHG	O8-C23-C24-C25
27	m	101	LMG	C33-C34-C35-C36
28	B	621	LHG	C32-C33-C34-C35
30	C	515	DGD	C2B-C3B-C4B-C5B
27	C	518	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	x	102	STE	C2-C3-C4-C5
30	C	516	DGD	O2G-C1B-C2B-C3B
22	b	614	CLA	CBA-CGA-O2A-C1
32	B	627	STE	O1-C1-C2-C3
29	A	412	SQD	C23-C24-C25-C26

There are no ring outliers.

116 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	510	CLA	2	0
24	c	514	BCR	2	0
22	b	615	CLA	3	0
32	D	412	STE	3	0
30	B	623	DGD	4	0
22	c	501	CLA	2	0
22	a	411	CLA	1	0
32	j	101	STE	1	0
22	a	405	CLA	1	0
27	d	408	LMG	1	0
29	L	101	SQD	2	0
30	c	515	DGD	1	0
22	B	614	CLA	2	0
28	L	102	LHG	6	0
24	B	617	BCR	1	0
27	c	520	LMG	1	0
22	c	512	CLA	1	0
24	B	618	BCR	2	0
27	A	410	LMG	3	0
29	A	412	SQD	4	0
28	l	101	LHG	1	0
32	H	103	STE	3	0
22	c	511	CLA	5	0
32	x	102	STE	2	0
26	a	410	PL9	3	0
22	b	606	CLA	2	0
22	C	510	CLA	1	0
30	A	414	DGD	3	0
32	b	625	STE	1	0
28	b	623	LHG	1	0
22	d	403	CLA	3	0
32	B	624	STE	2	0

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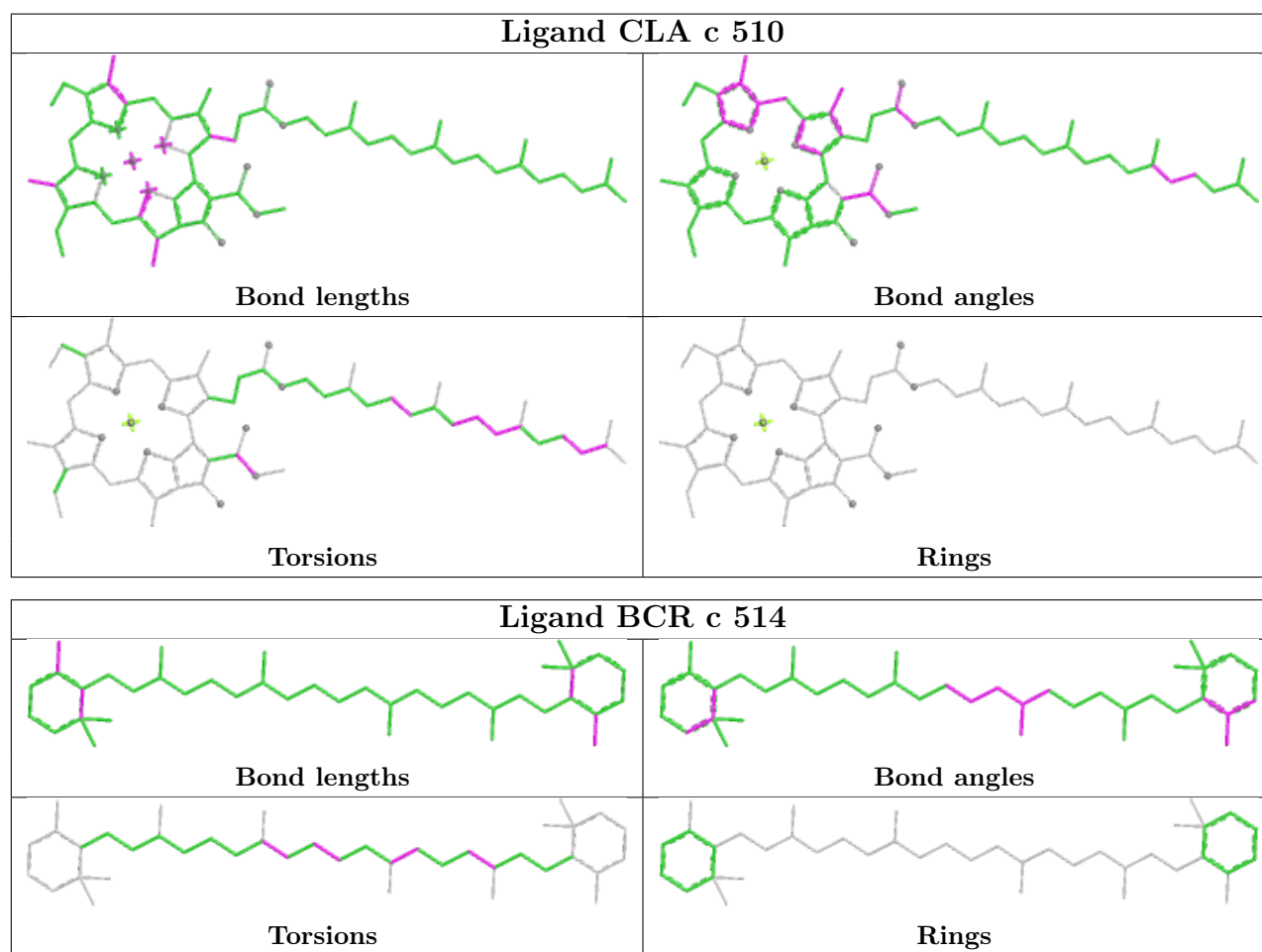
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	619	BCR	1	0
28	d	406	LHG	3	0
22	B	606	CLA	3	0
26	A	409	PL9	3	0
22	b	604	CLA	1	0
22	C	507	CLA	1	0
22	c	513	CLA	1	0
24	C	514	BCR	1	0
22	B	609	CLA	1	0
34	F	101	HEM	2	0
26	D	407	PL9	1	0
22	b	601	CLA	2	0
28	E	101	LHG	2	0
24	t	101	BCR	3	0
28	B	621	LHG	4	0
32	J	101	STE	1	0
35	V	201	HEC	1	0
22	B	604	CLA	2	0
28	D	409	LHG	2	0
24	d	404	BCR	3	0
29	a	413	SQD	2	0
22	C	509	CLA	2	0
22	C	502	CLA	1	0
30	C	516	DGD	4	0
30	c	517	DGD	2	0
22	B	611	CLA	3	0
32	M	104	STE	1	0
29	a	412	SQD	4	0
22	c	503	CLA	3	0
22	b	607	CLA	1	0
22	C	511	CLA	2	0
22	d	402	CLA	1	0
22	B	603	CLA	2	0
22	b	616	CLA	2	0
22	c	508	CLA	1	0
32	l	102	STE	1	0
22	B	602	CLA	2	0
24	Z	101	BCR	2	0
30	C	517	DGD	2	0
27	M	101	LMG	1	0
22	B	605	CLA	4	0
24	K	101	BCR	2	0

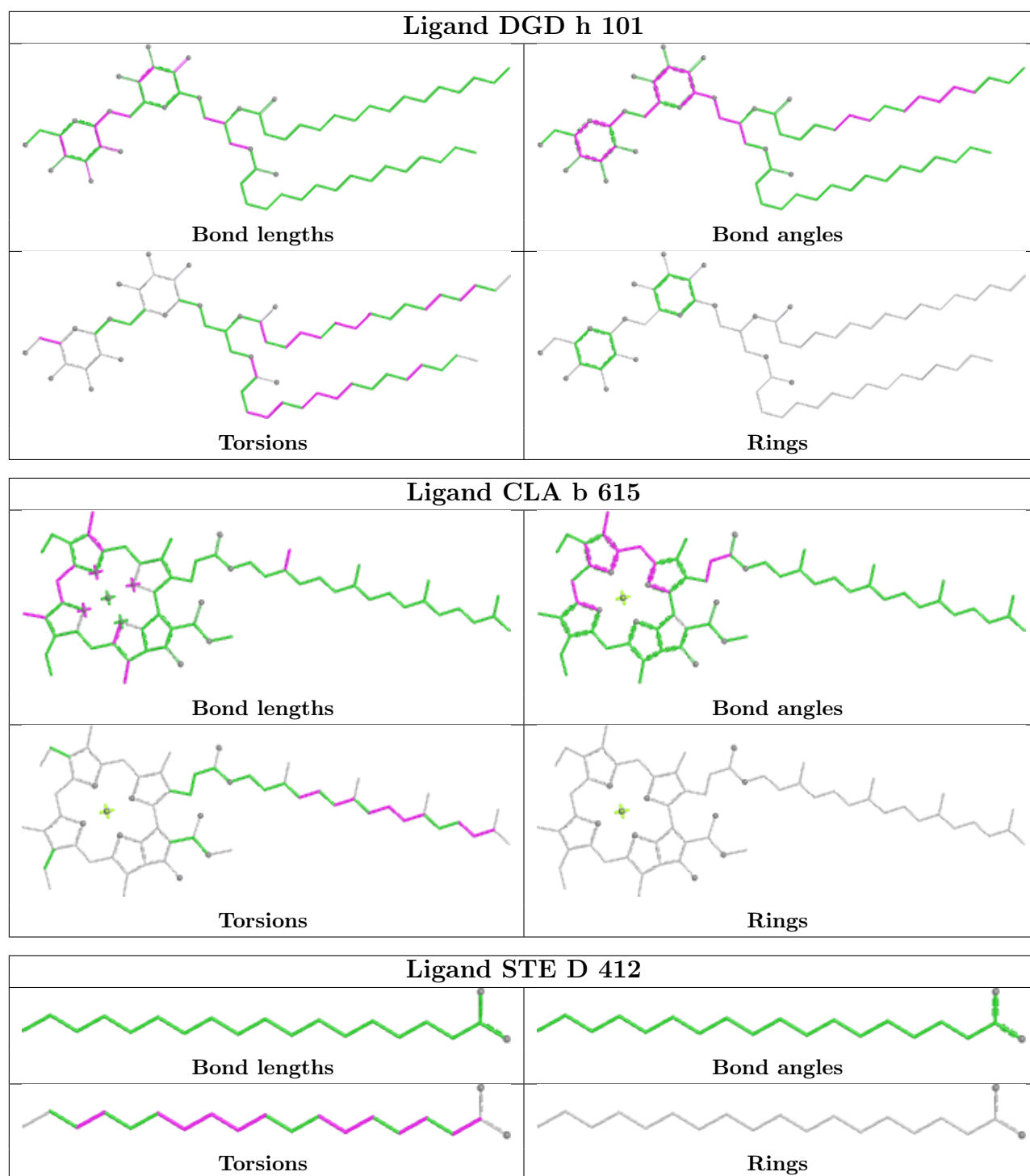
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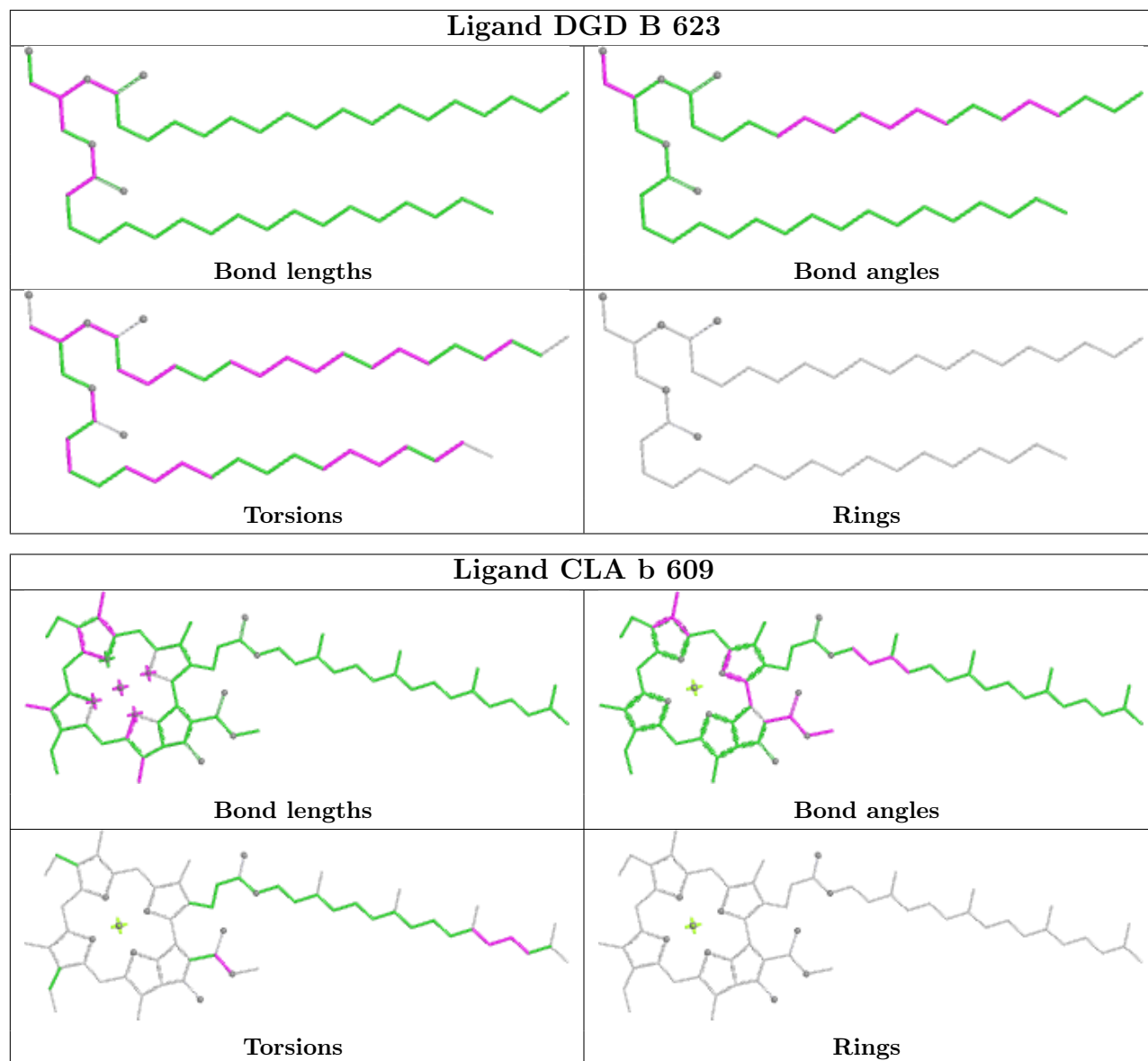
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	502	CLA	1	0
32	b	626	STE	1	0
24	D	406	BCR	1	0
28	e	102	LHG	3	0
22	A	402	CLA	1	0
22	b	602	CLA	1	0
24	x	101	BCR	1	0
27	C	518	LMG	1	0
27	D	408	LMG	1	0
32	I	101	STE	1	0
22	B	615	CLA	1	0
30	c	516	DGD	2	0
22	b	614	CLA	2	0
24	b	617	BCR	1	0
22	C	504	CLA	1	0
22	b	605	CLA	2	0
32	b	624	STE	1	0
34	e	101	HEM	4	0
22	D	404	CLA	3	0
23	d	401	PHO	1	0
24	b	618	BCR	1	0
22	A	403	CLA	1	0
28	d	407	LHG	2	0
29	A	413	SQD	1	0
24	T	101	BCR	3	0
33	D	402	BCT	1	0
32	b	620	STE	1	0
23	a	404	PHO	1	0
32	k	104	STE	2	0
22	b	610	CLA	2	0
22	c	507	CLA	1	0
29	B	622	SQD	1	0
30	H	102	DGD	1	0
32	B	627	STE	2	0
24	a	406	BCR	1	0
22	B	601	CLA	3	0
23	D	401	PHO	1	0
32	B	620	STE	1	0
22	B	613	CLA	3	0
28	A	411	LHG	2	0
29	f	101	SQD	2	0
32	b	621	STE	1	0

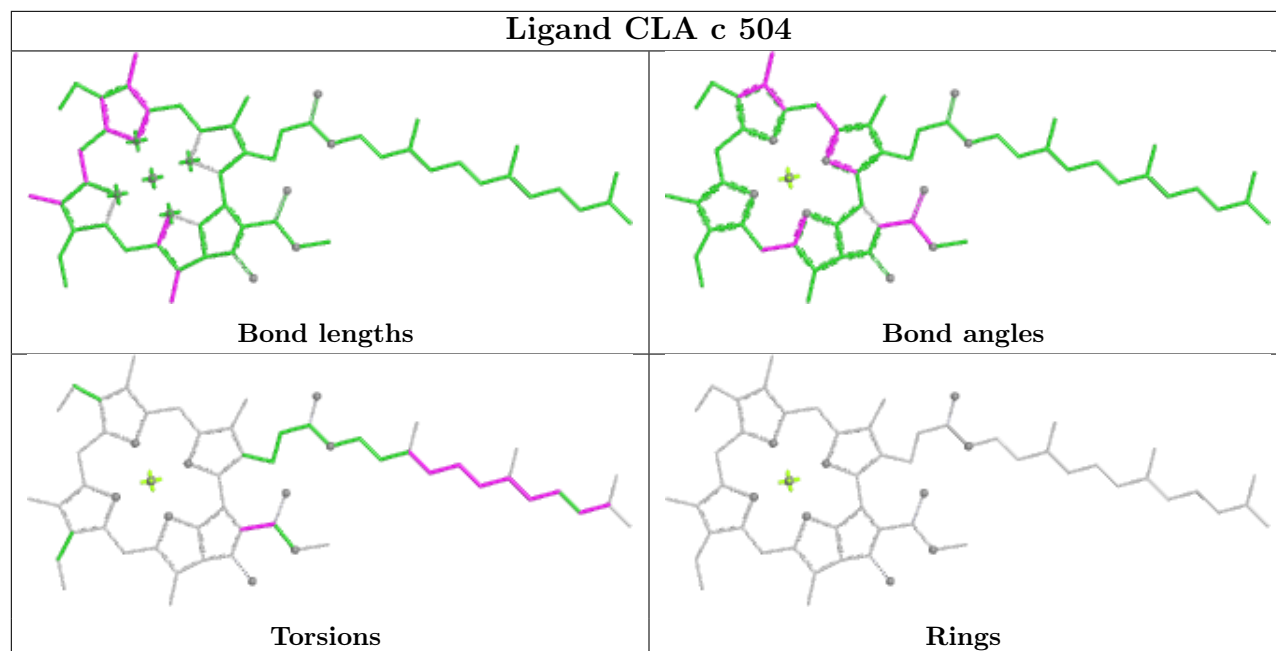
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



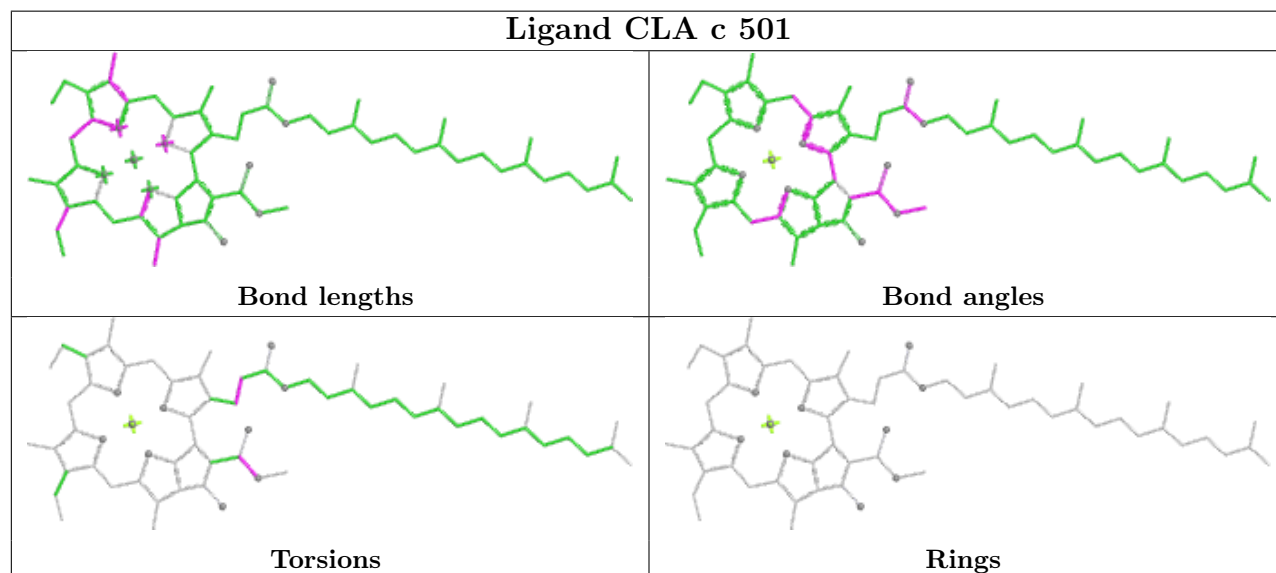


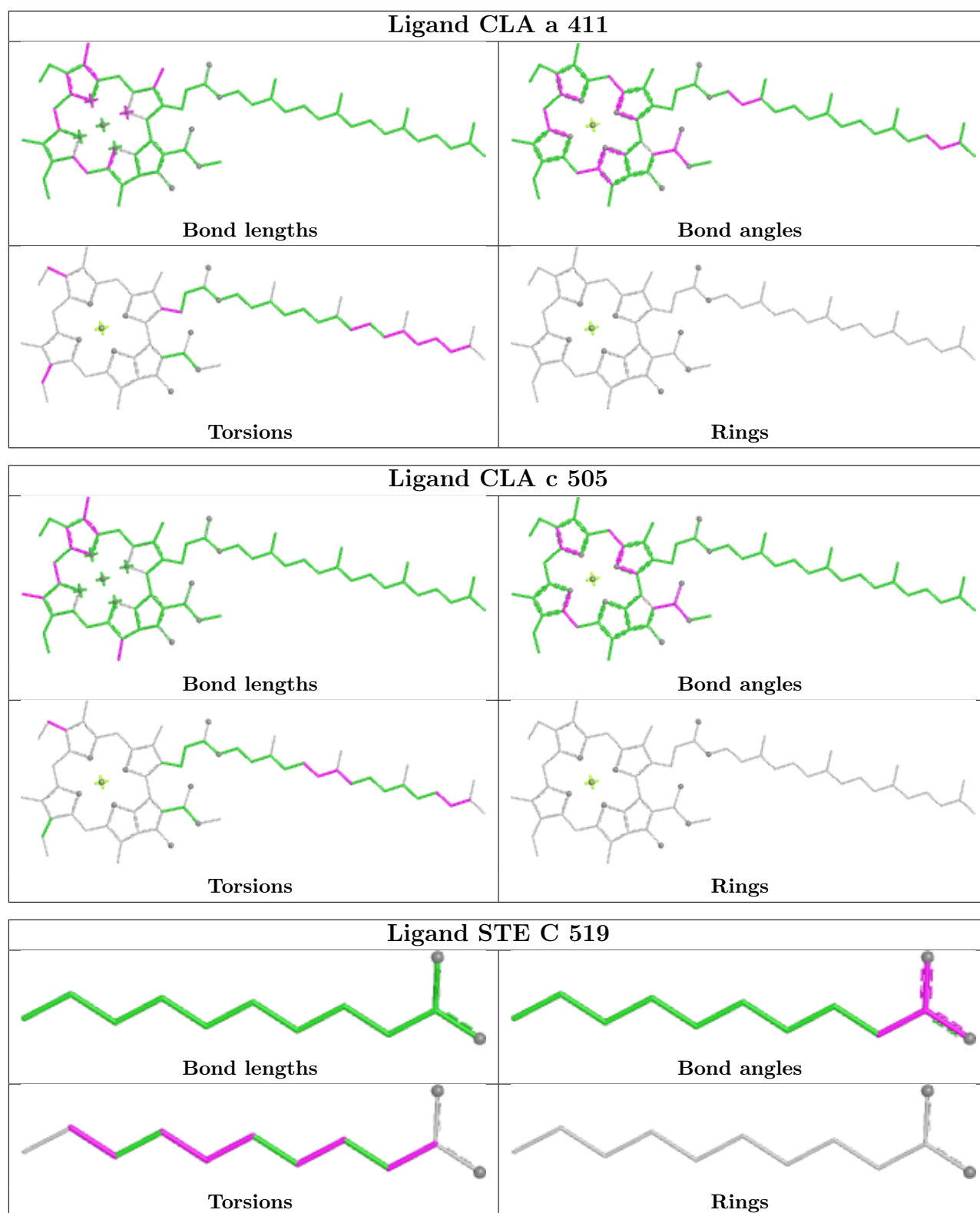


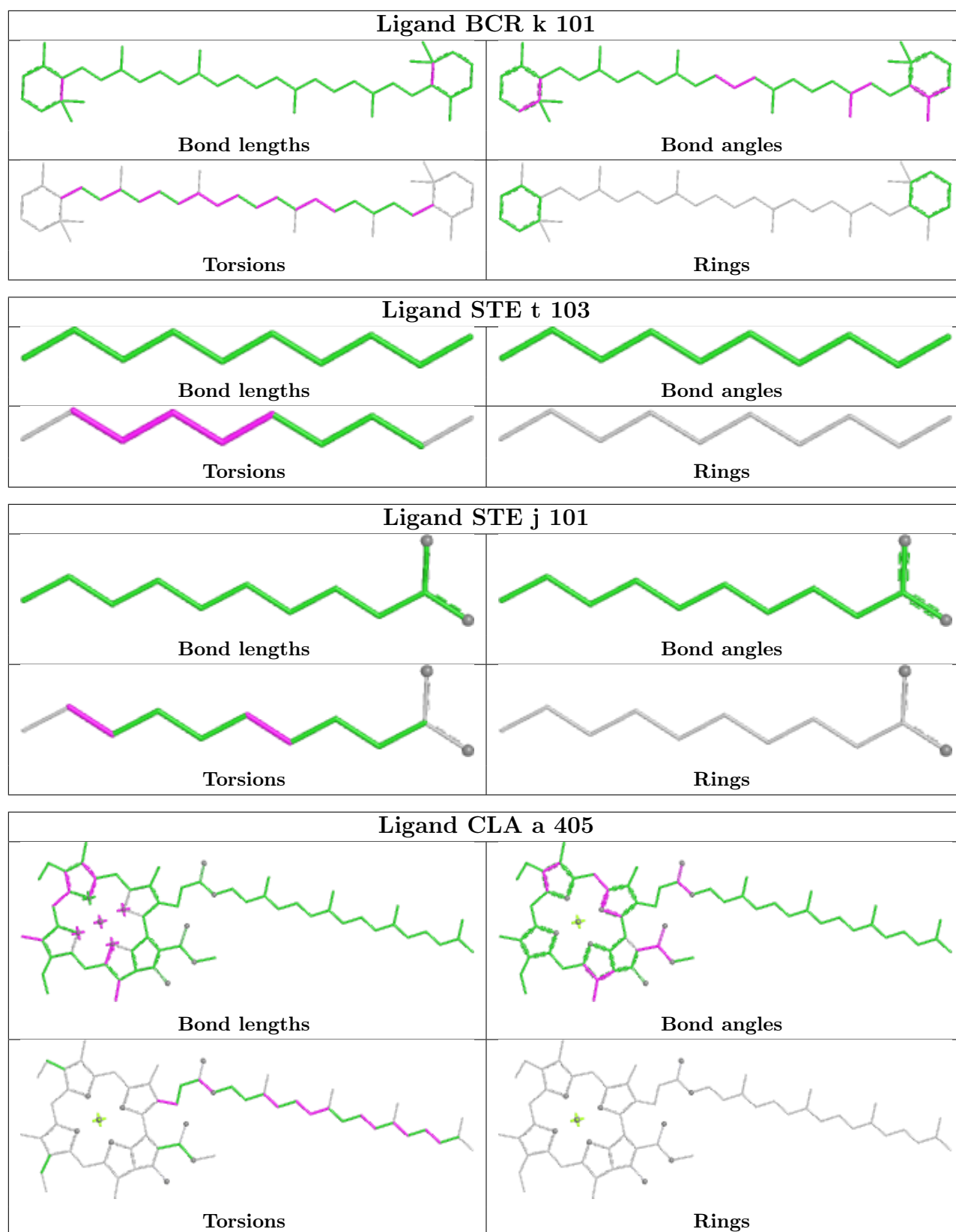
Ligand CLA c 504

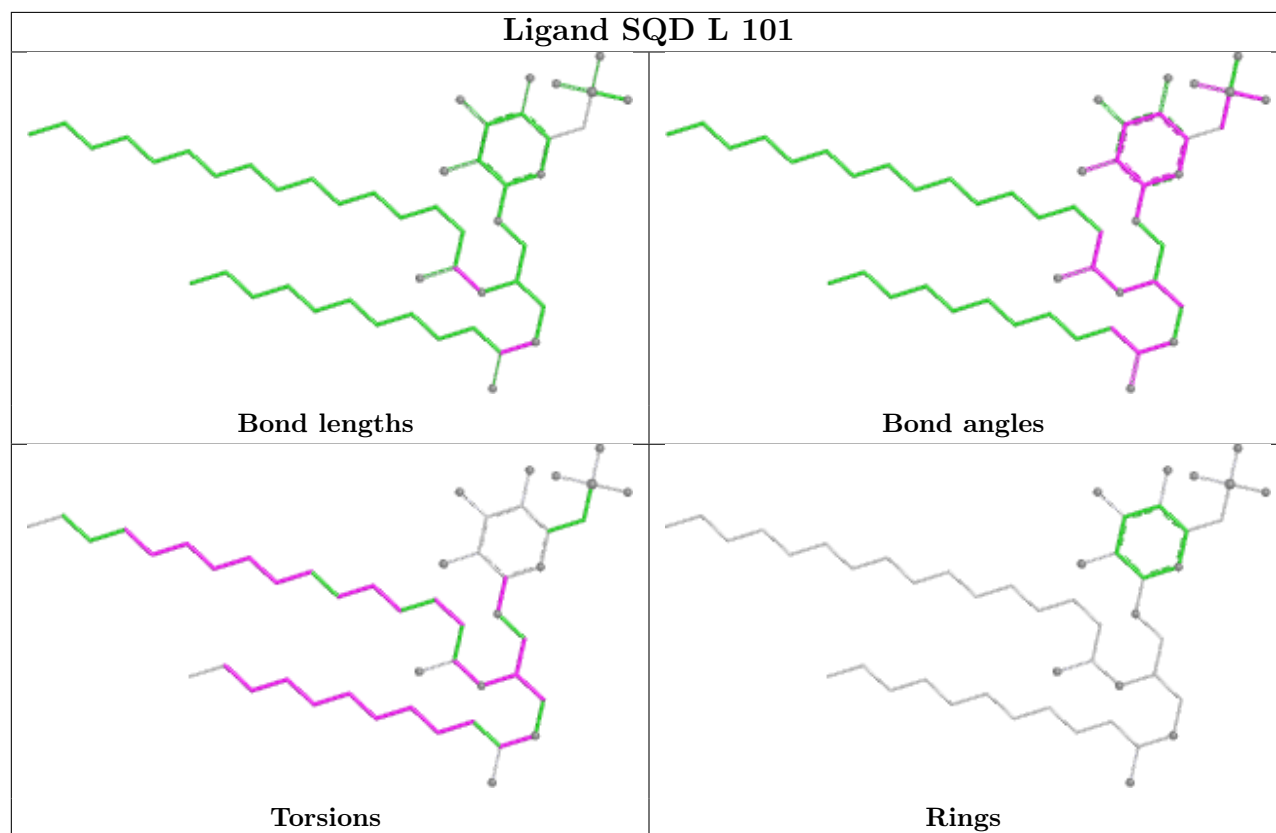
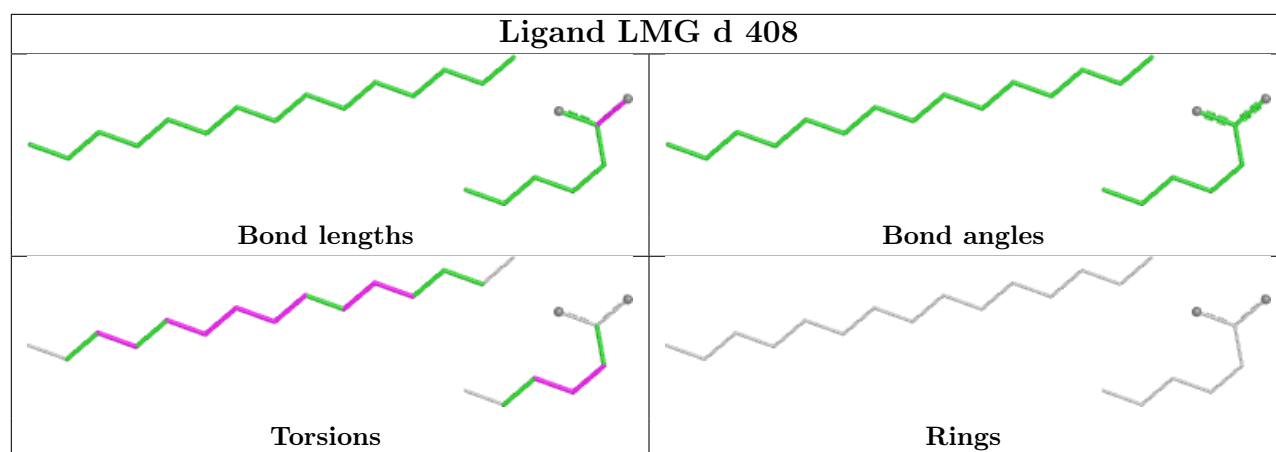


Ligand CLA c 501

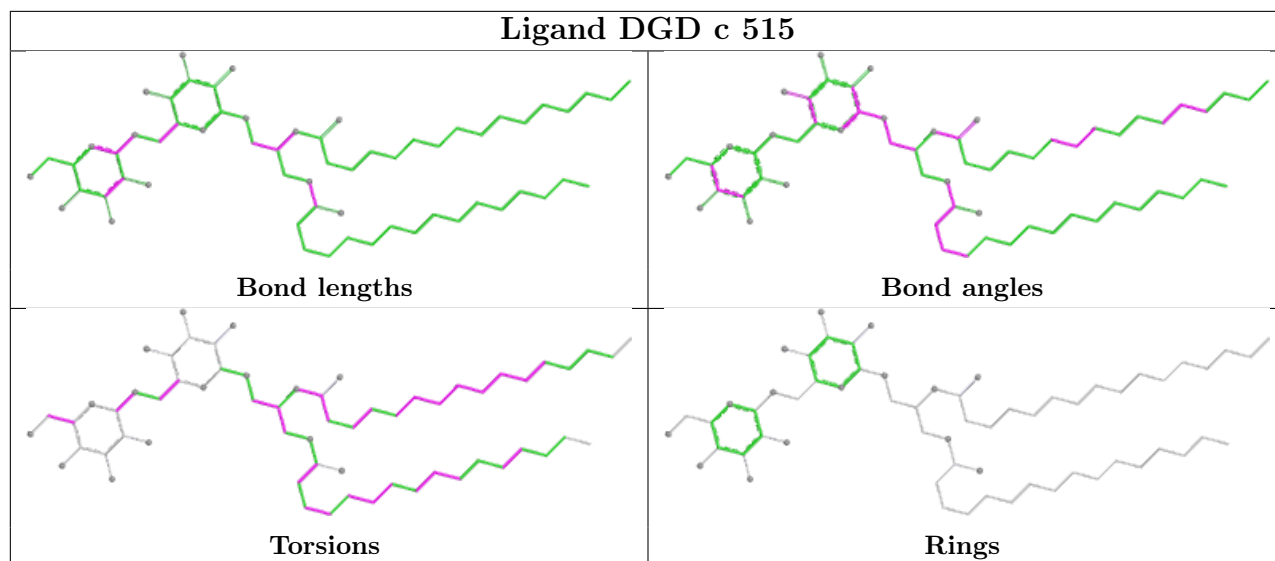




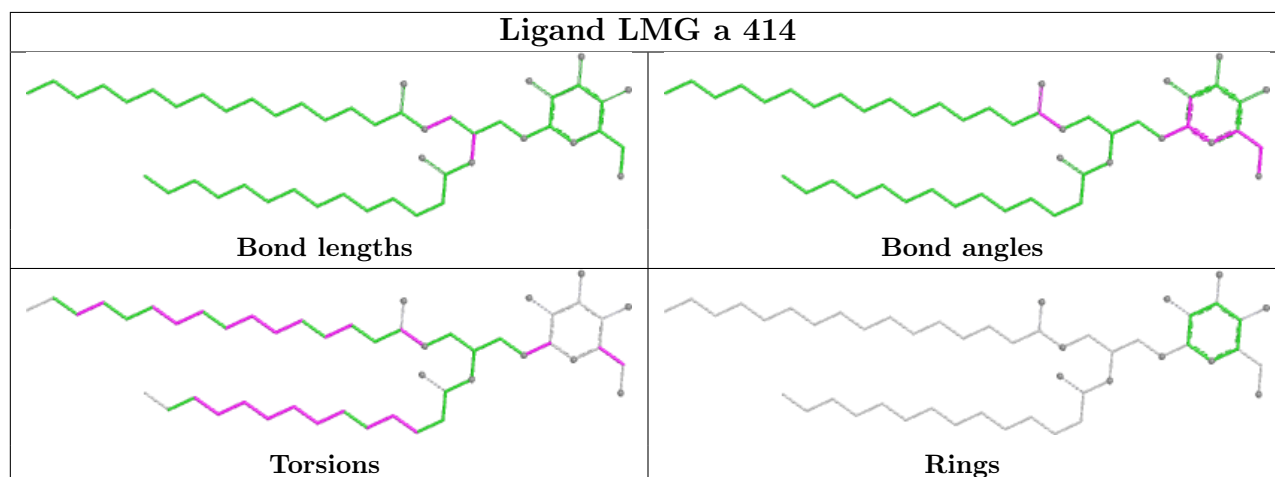




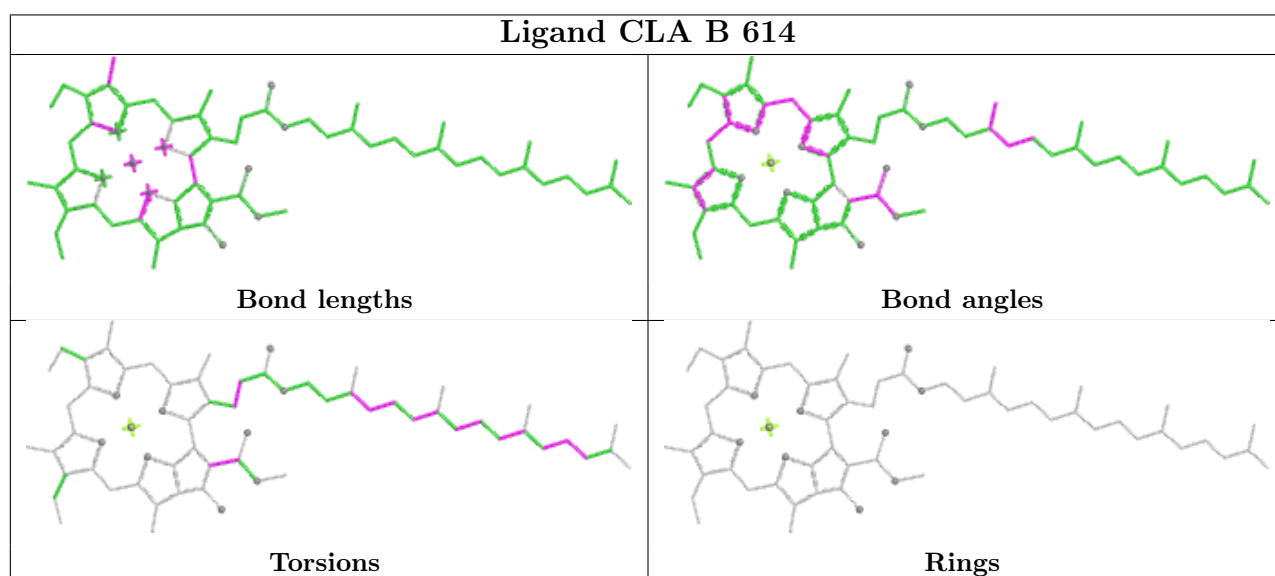
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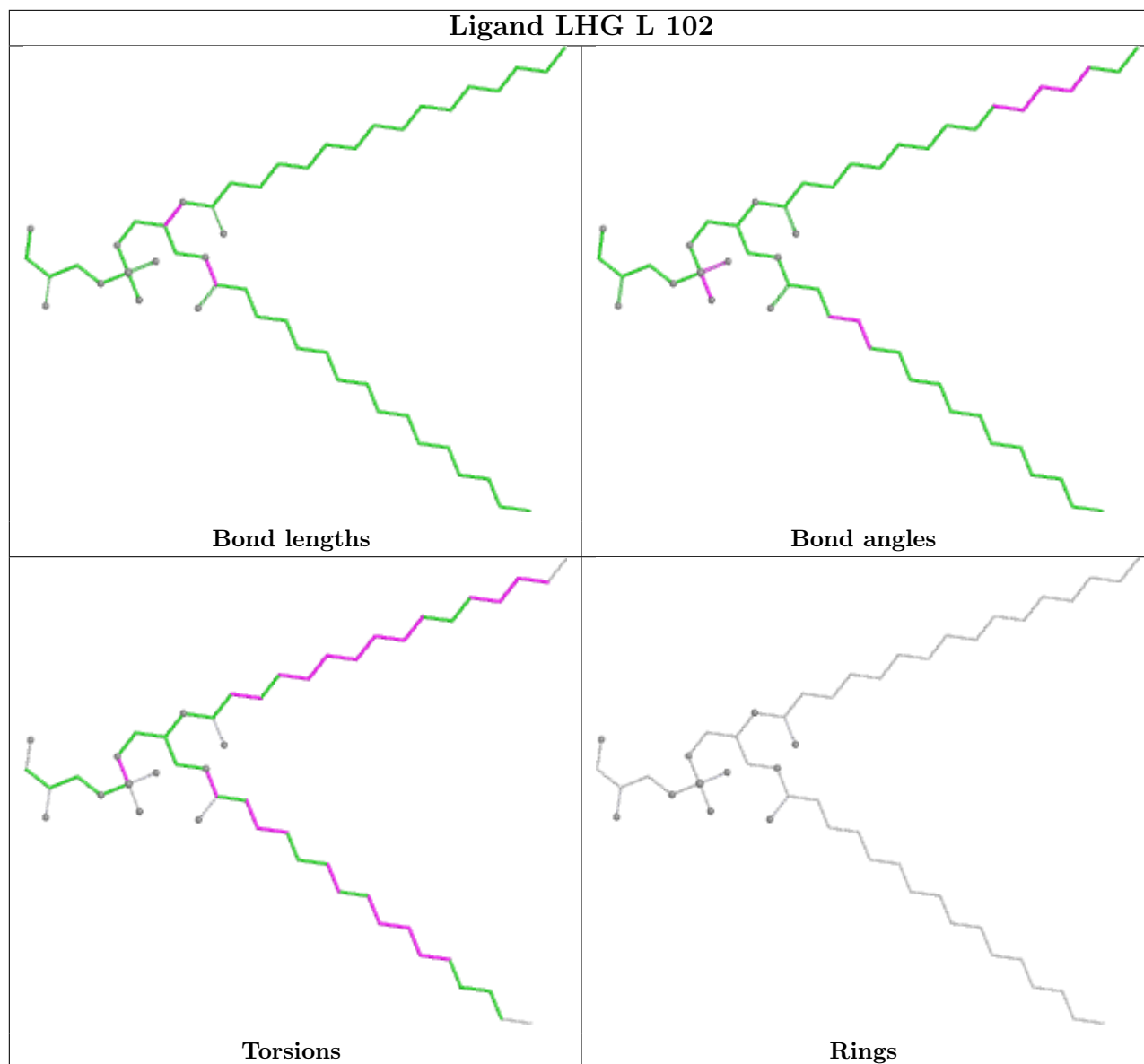
Ligand LMG a 414



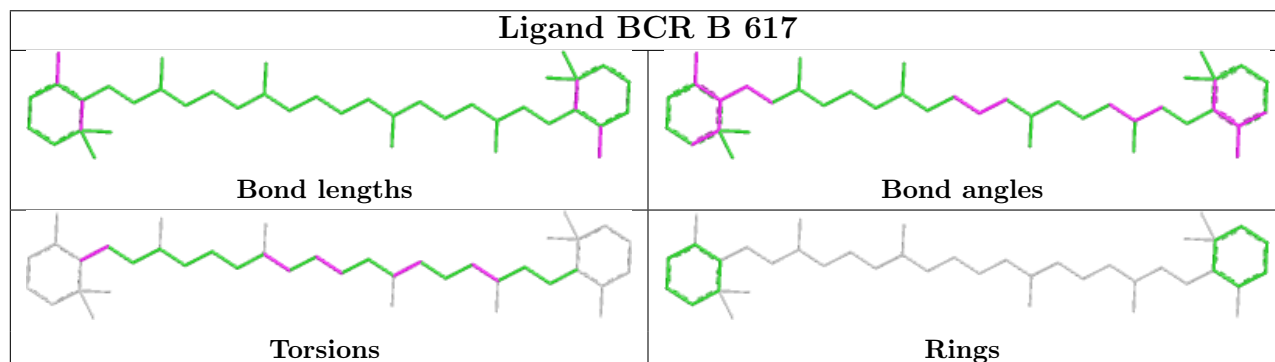
Ligand CLA B 614

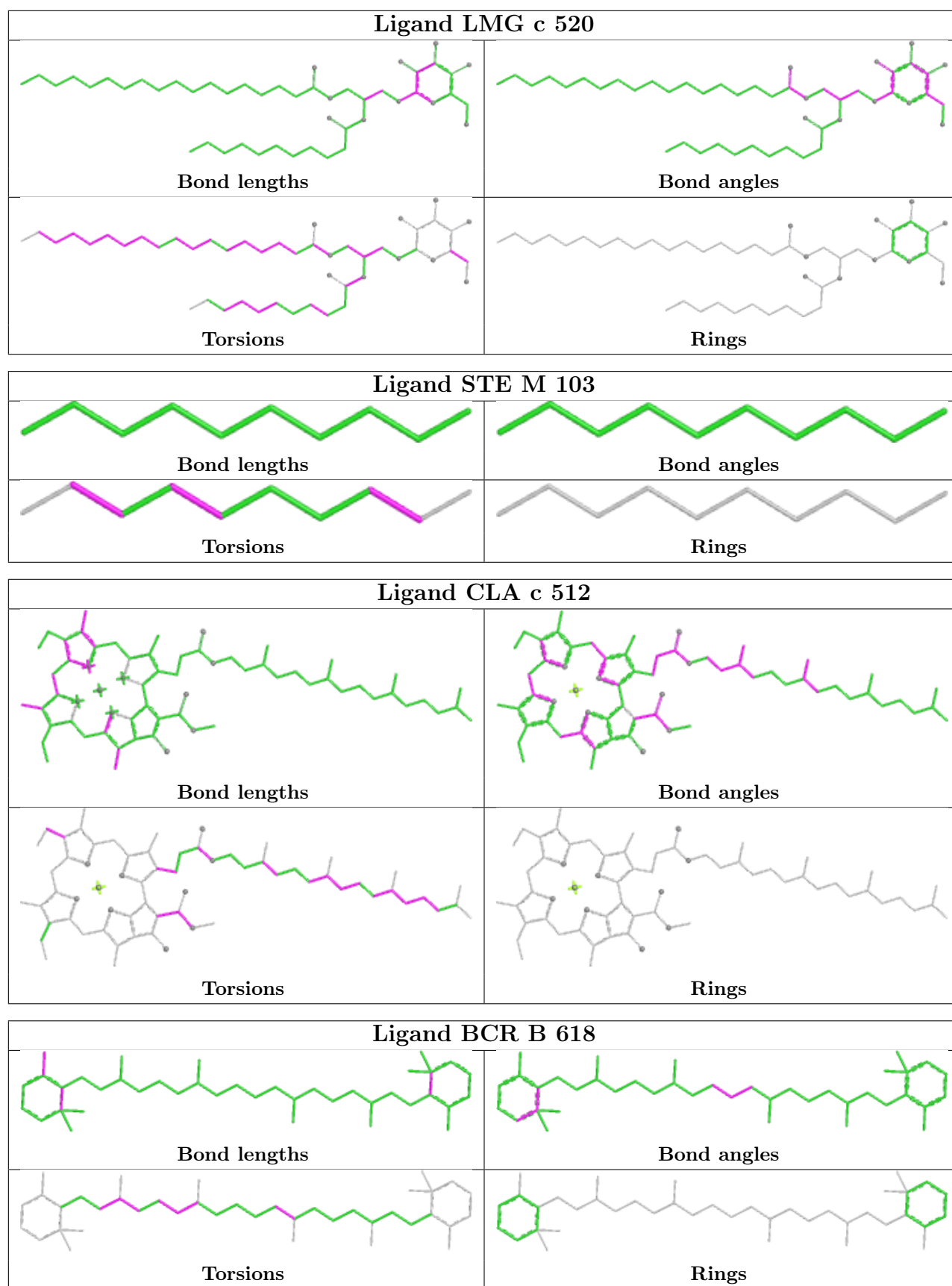


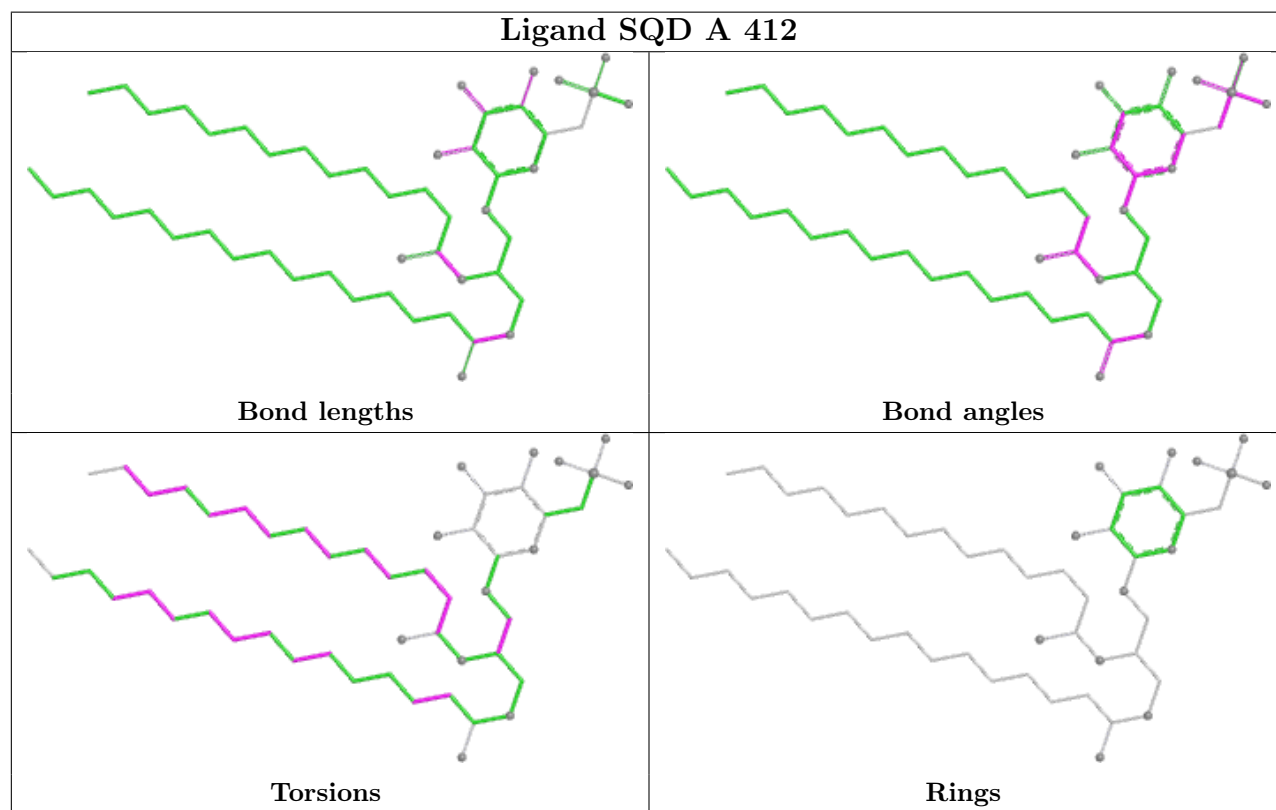
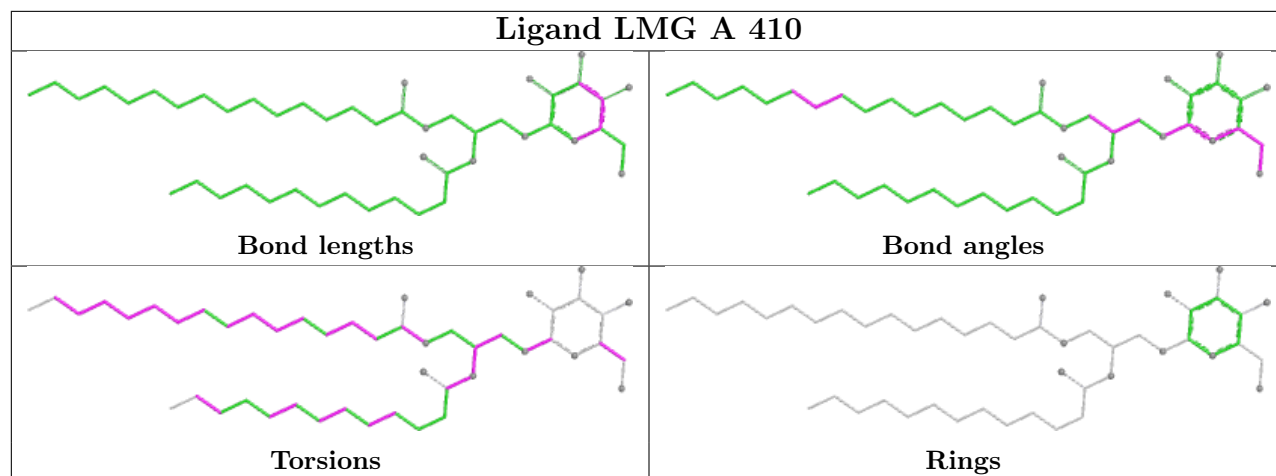
Ligand LHG L 102

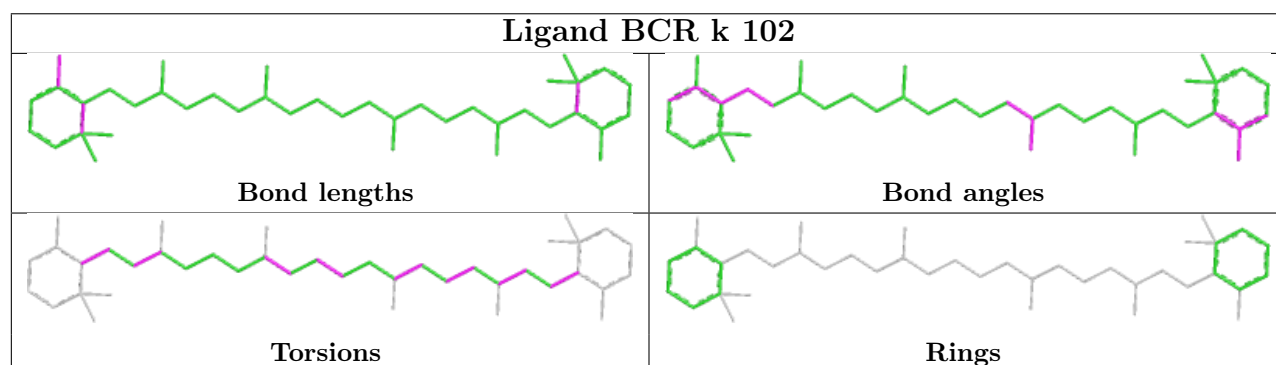
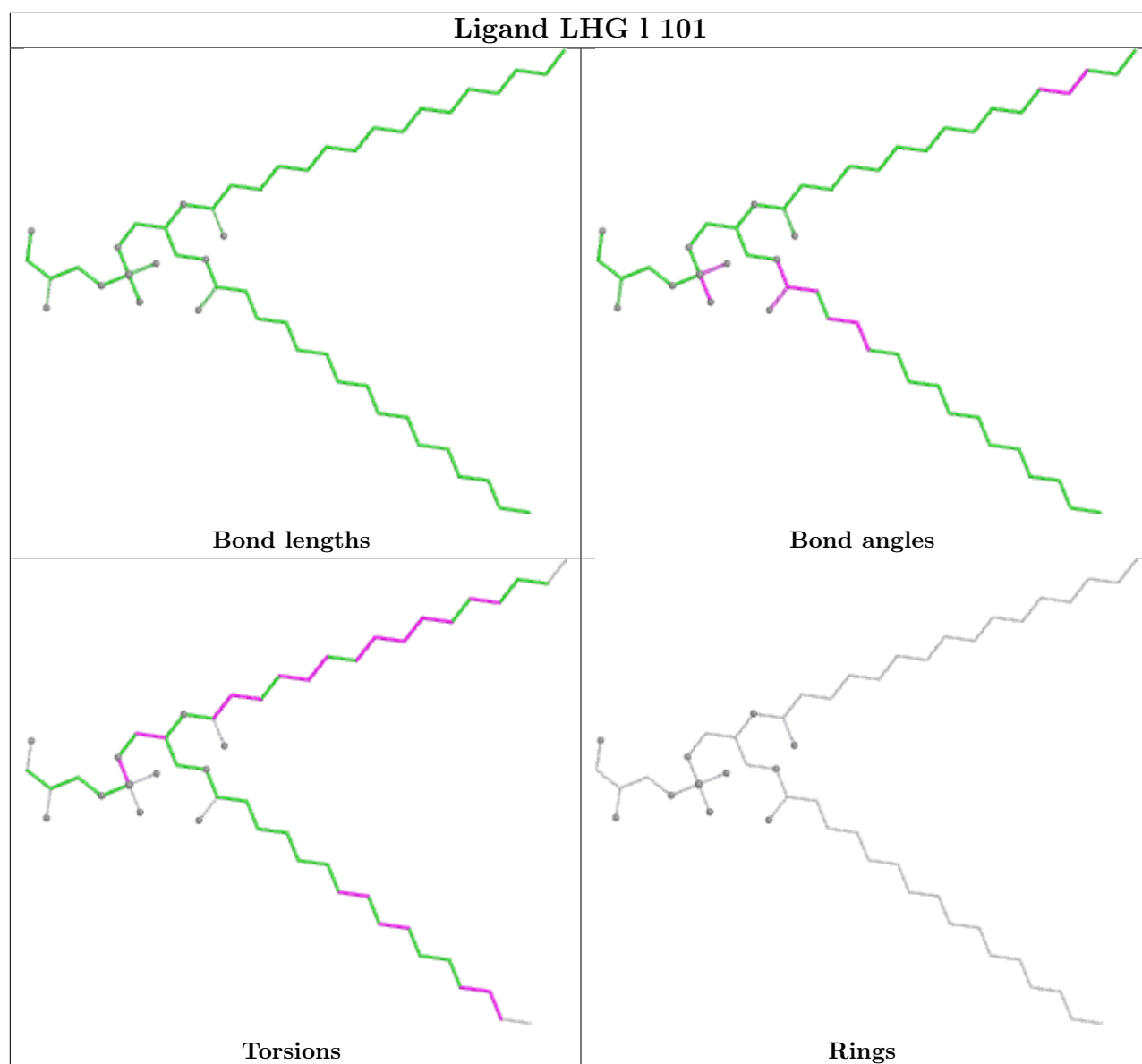


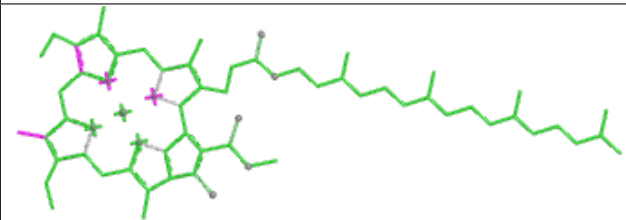
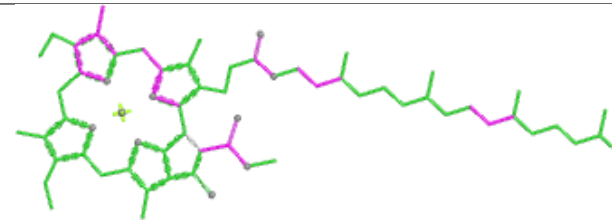
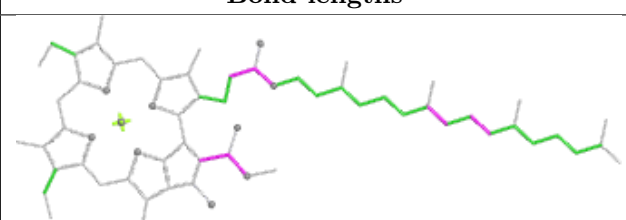
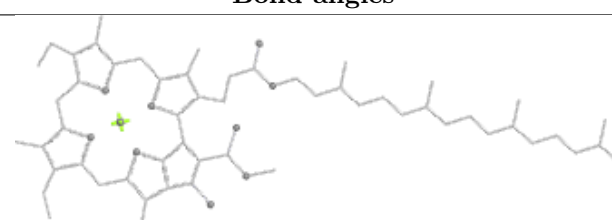
Ligand BCR B 617



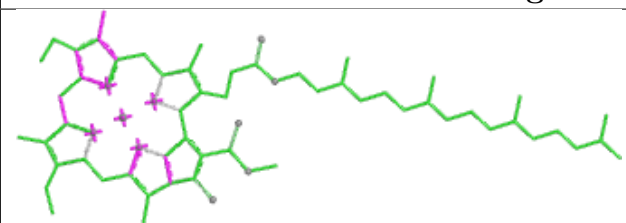
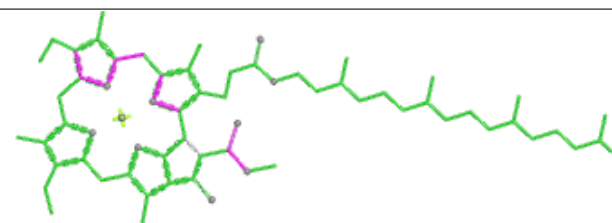
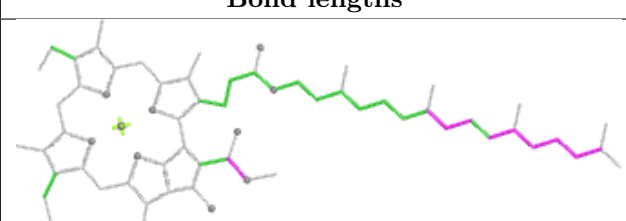
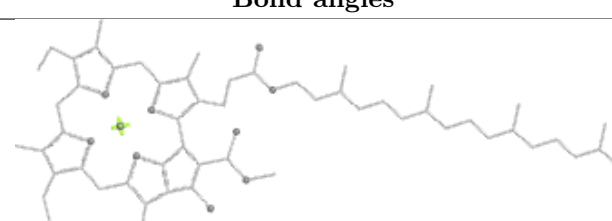


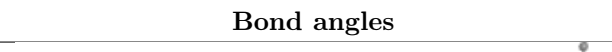


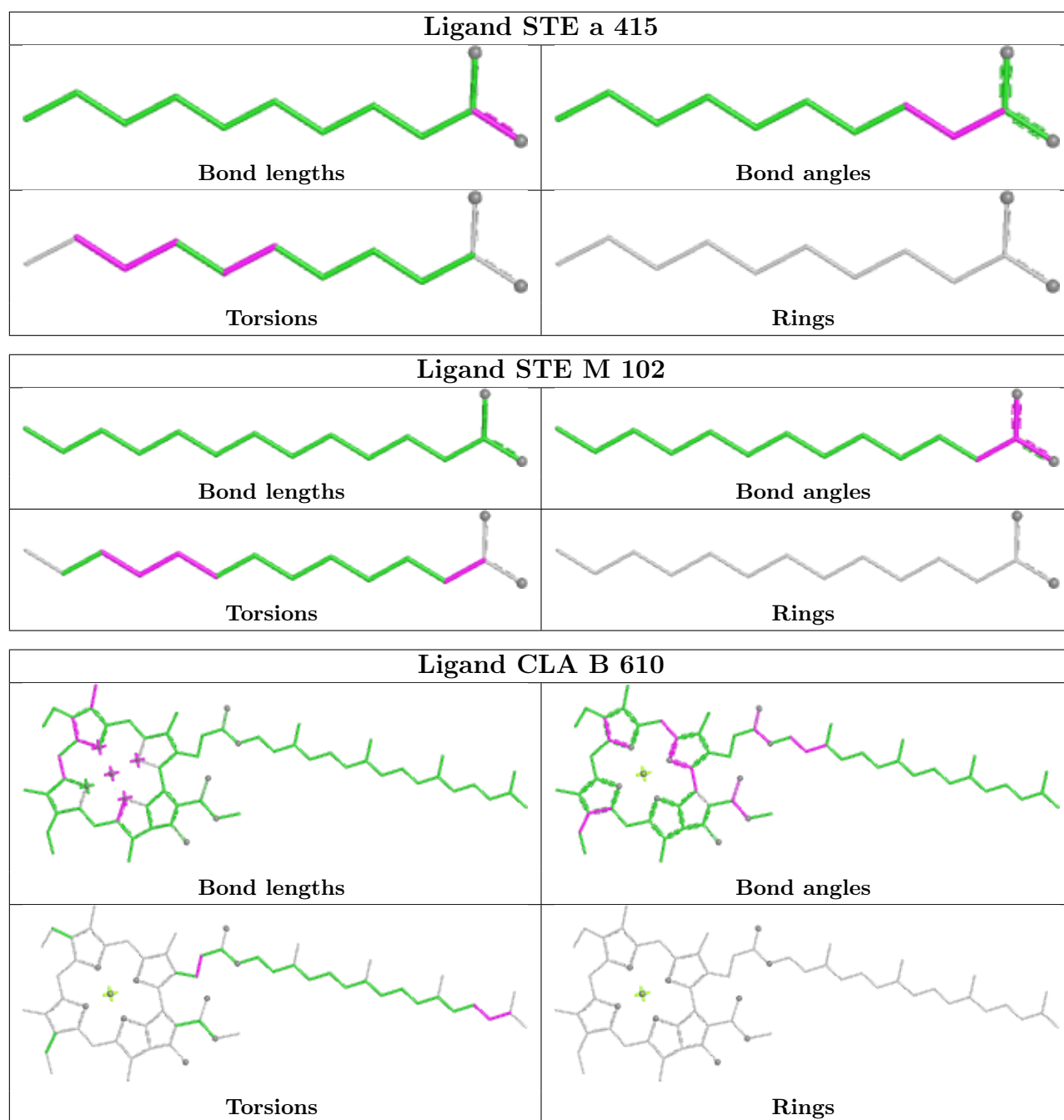


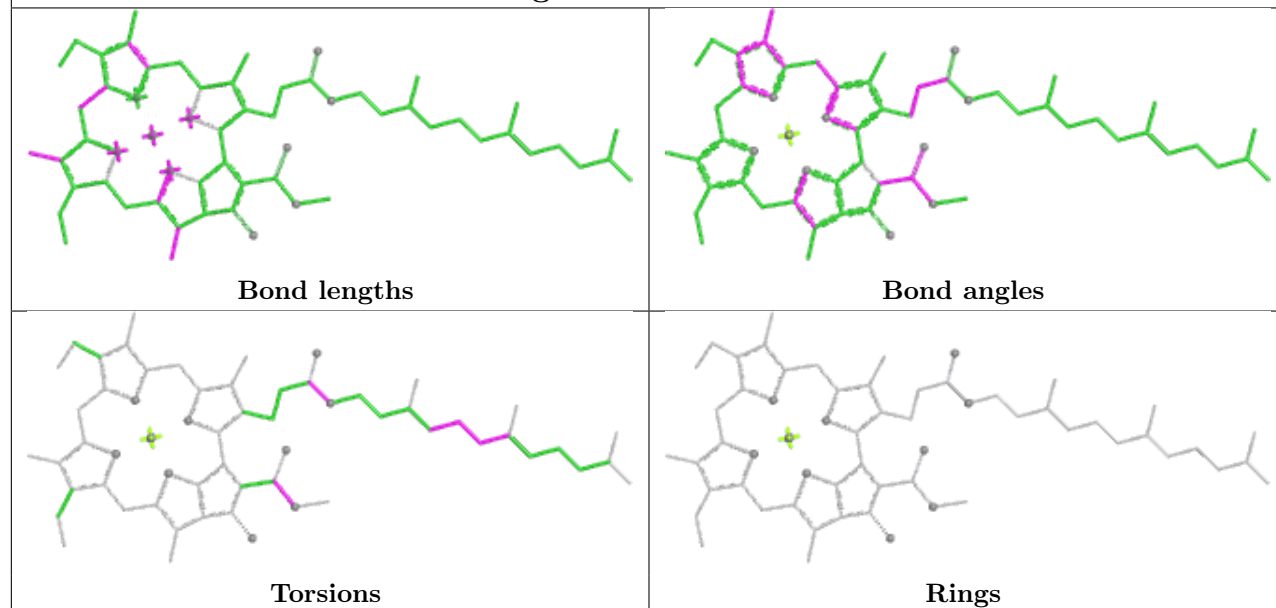
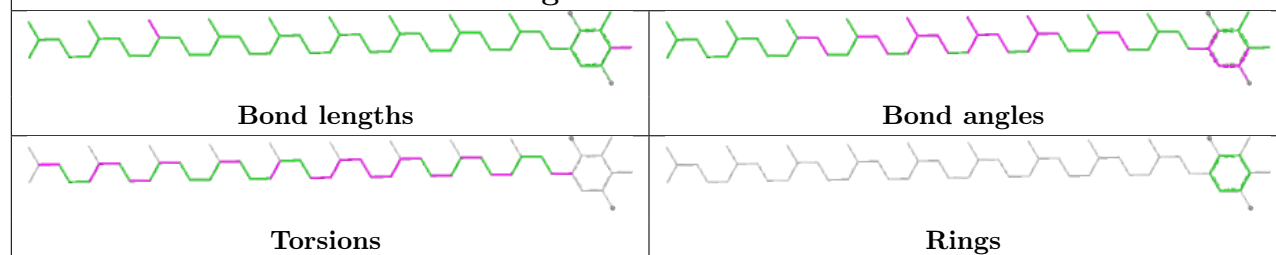
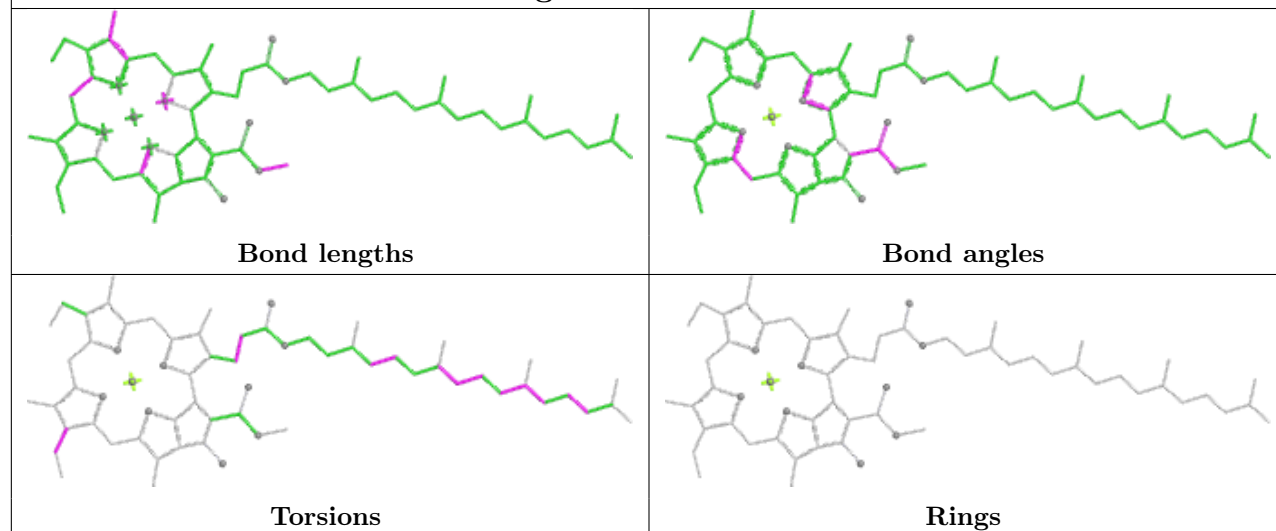
Ligand CLA B 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

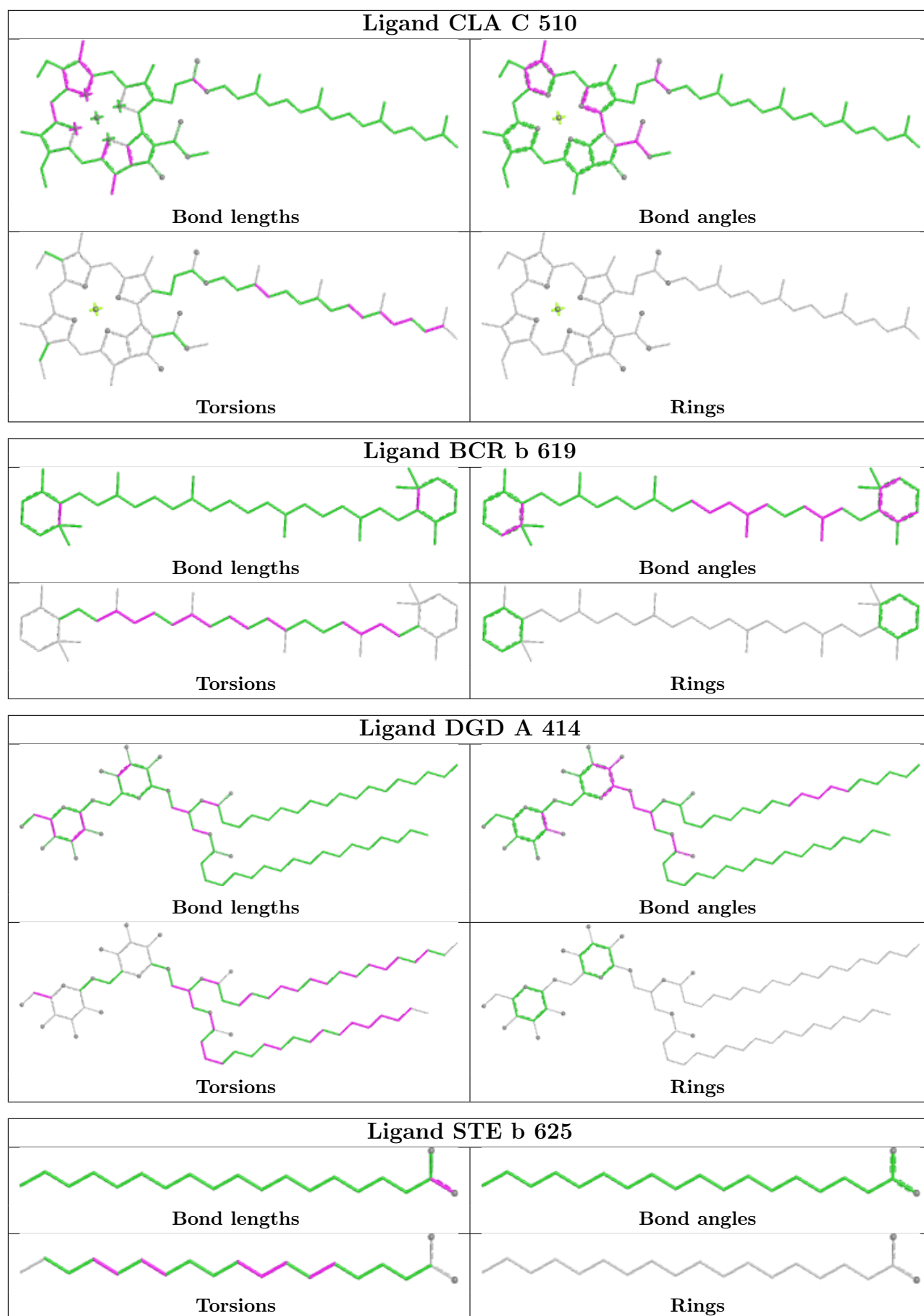
Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

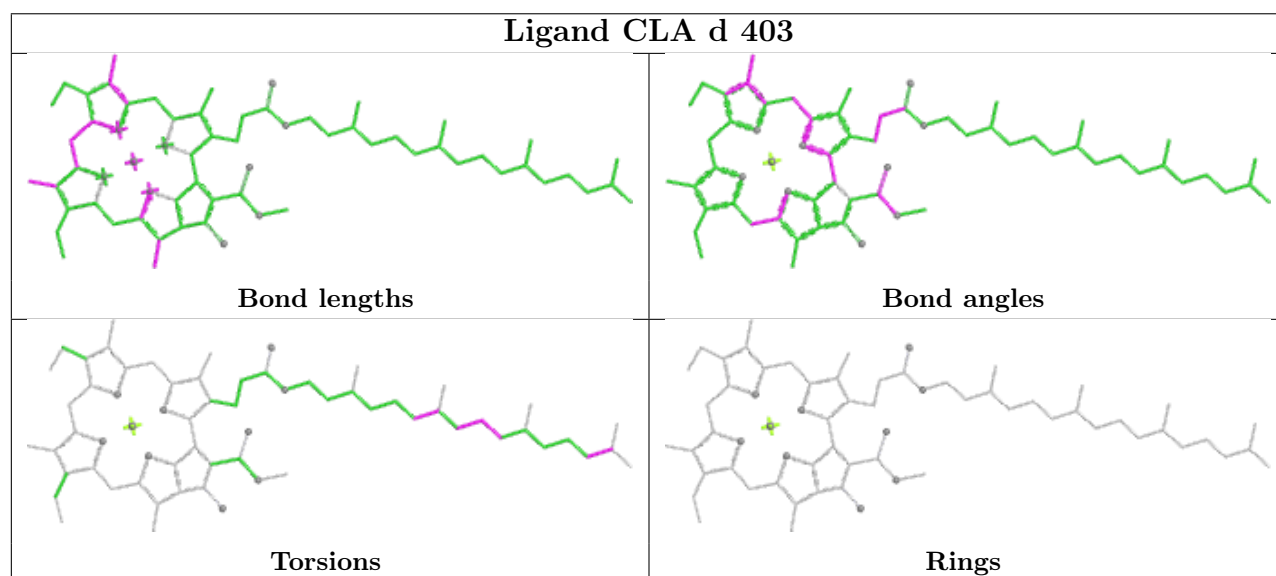
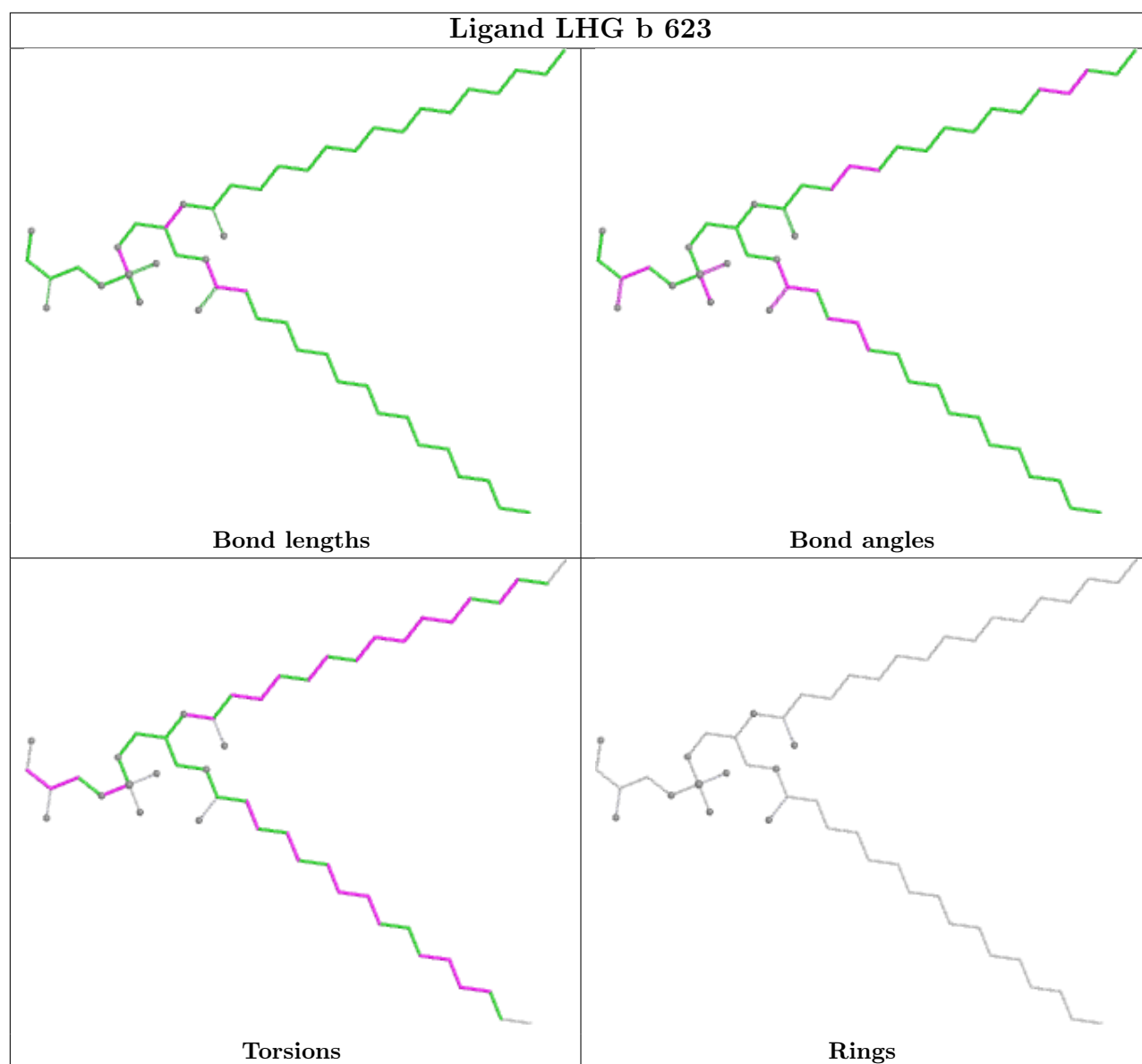
Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

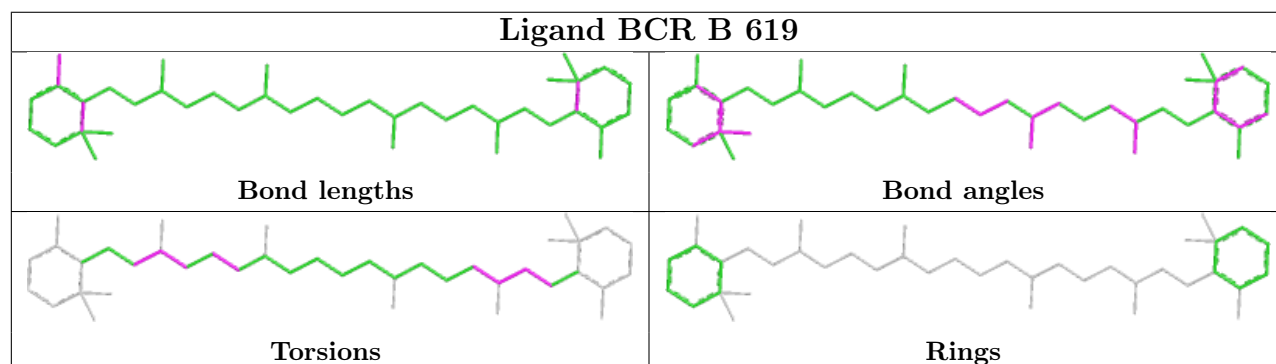
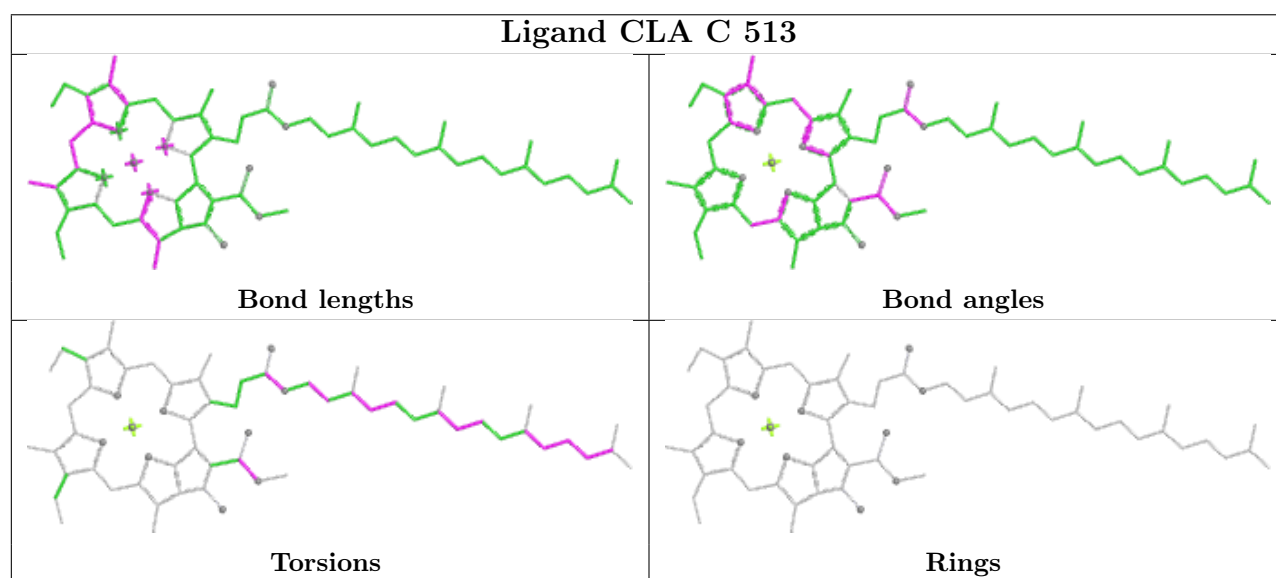
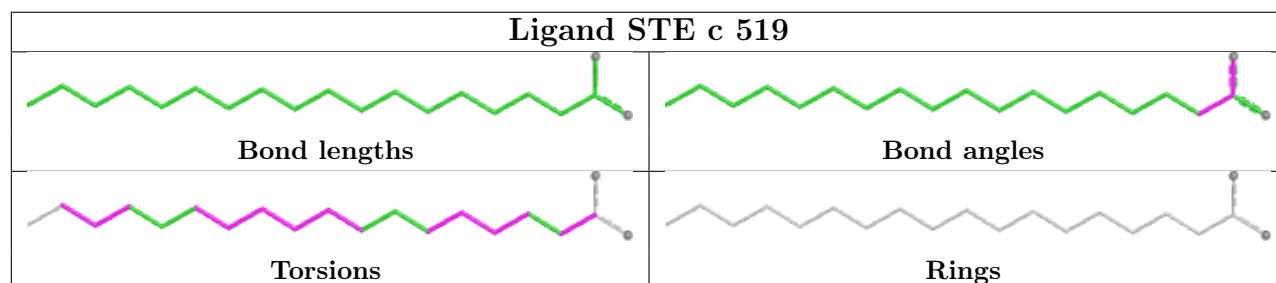
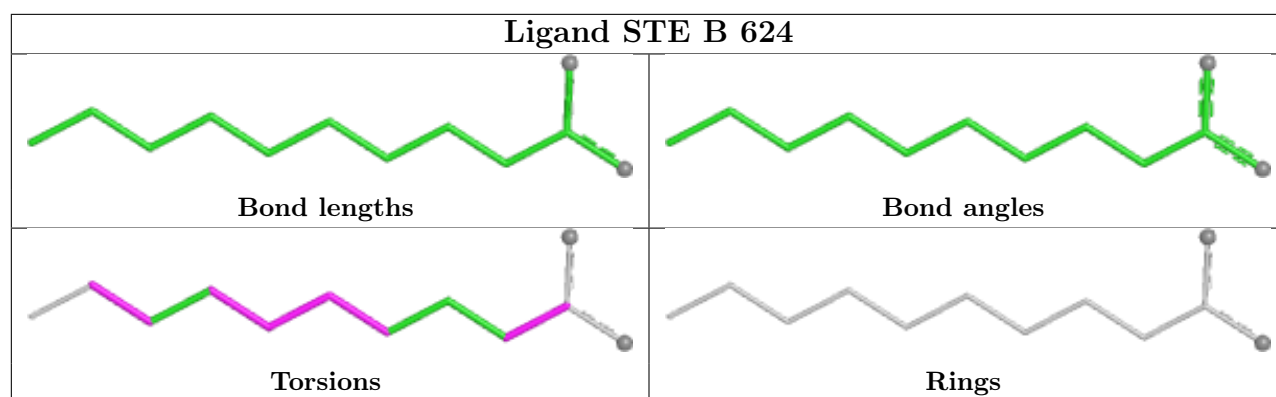
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Bond lengths	Bond angles
	
Torsions	Rings



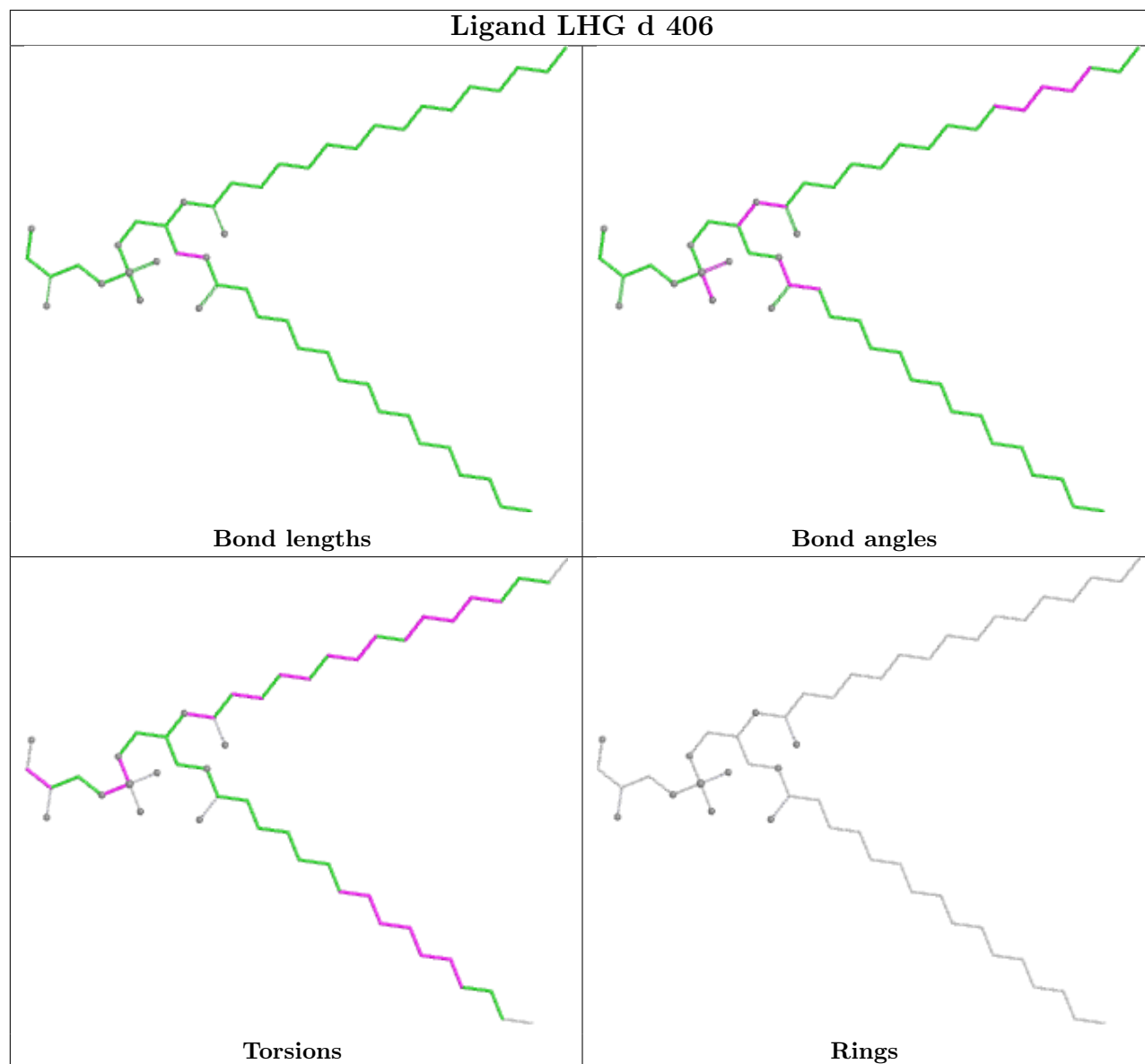
Ligand CLA B 616**Ligand PL9 a 410****Ligand CLA b 606**



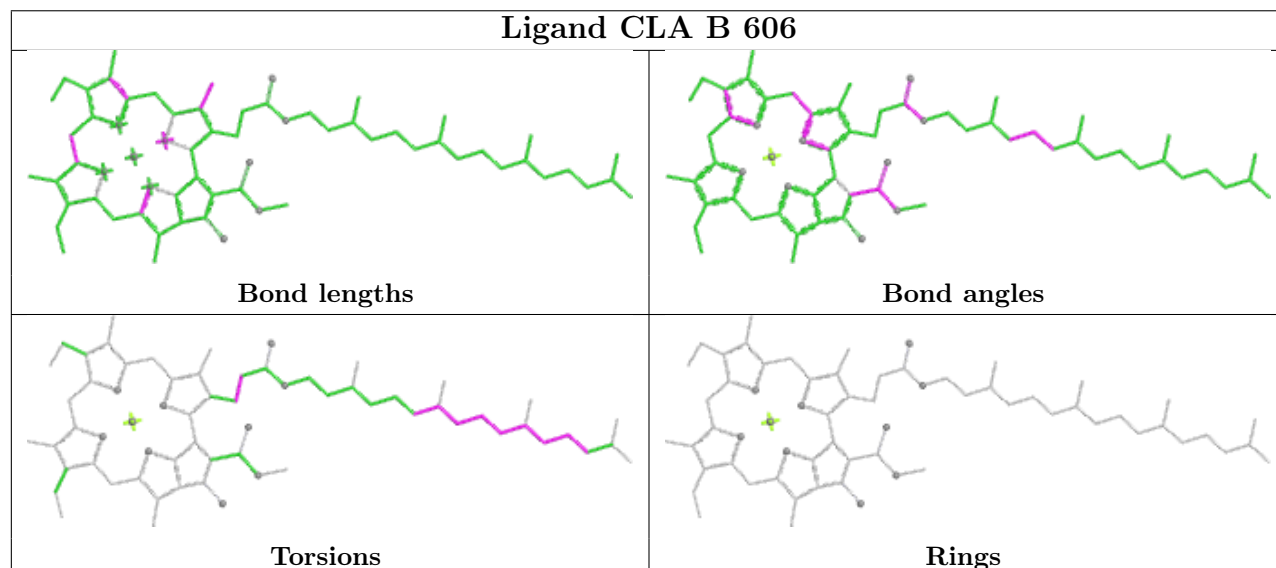


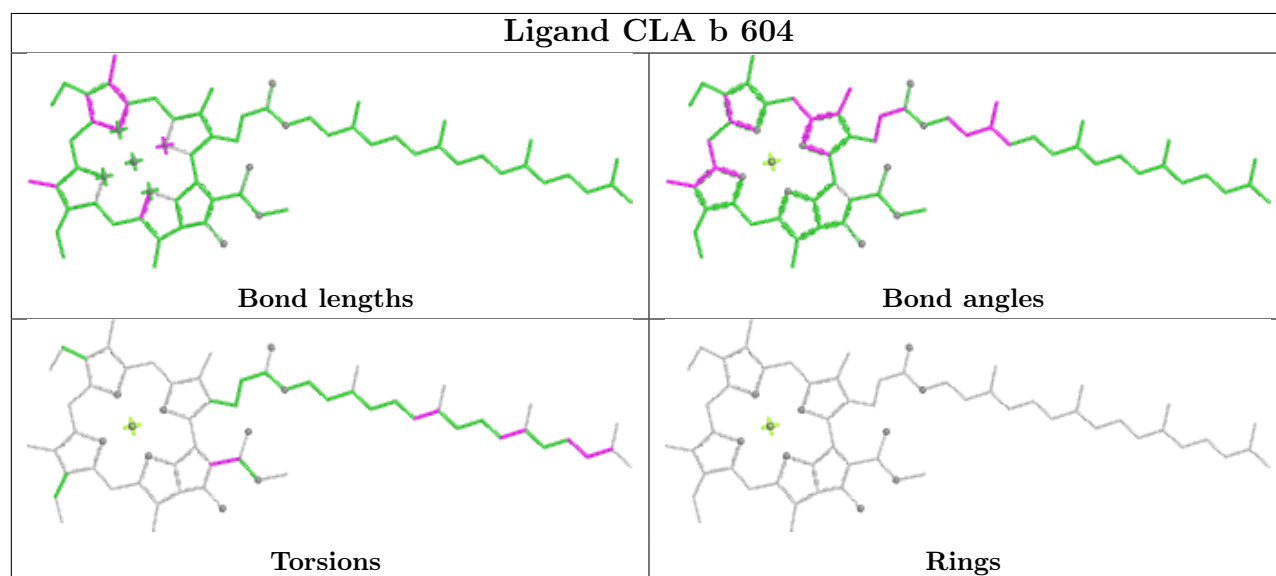
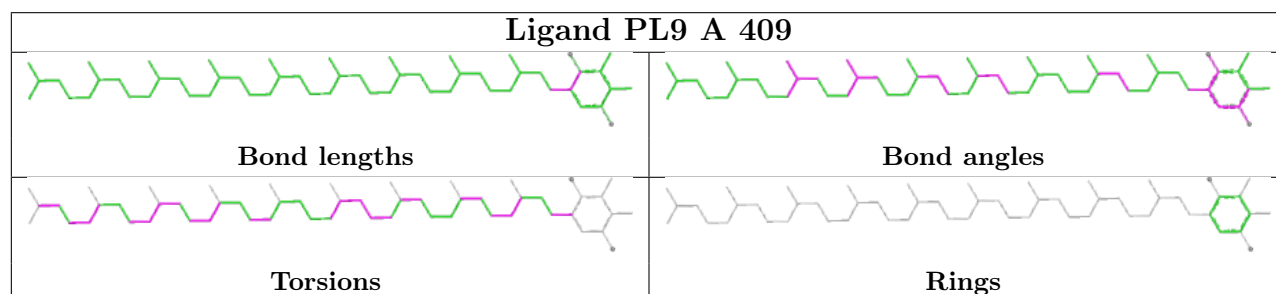
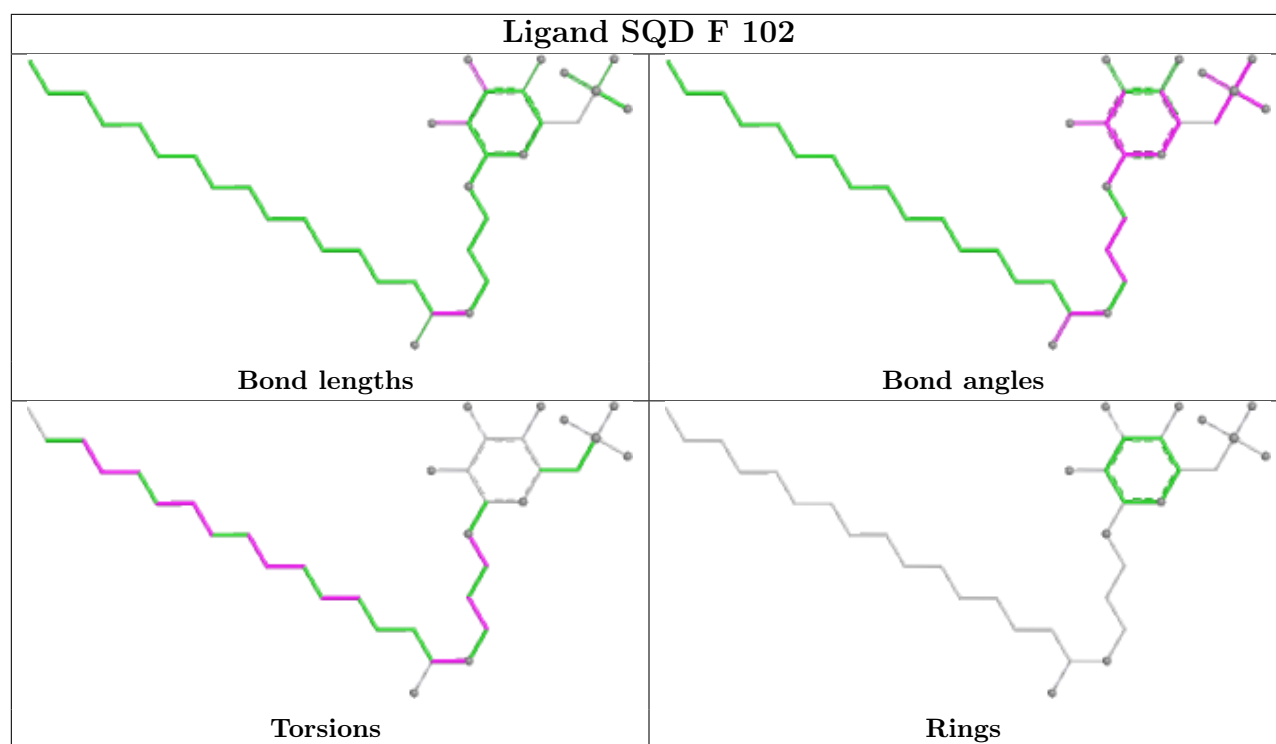


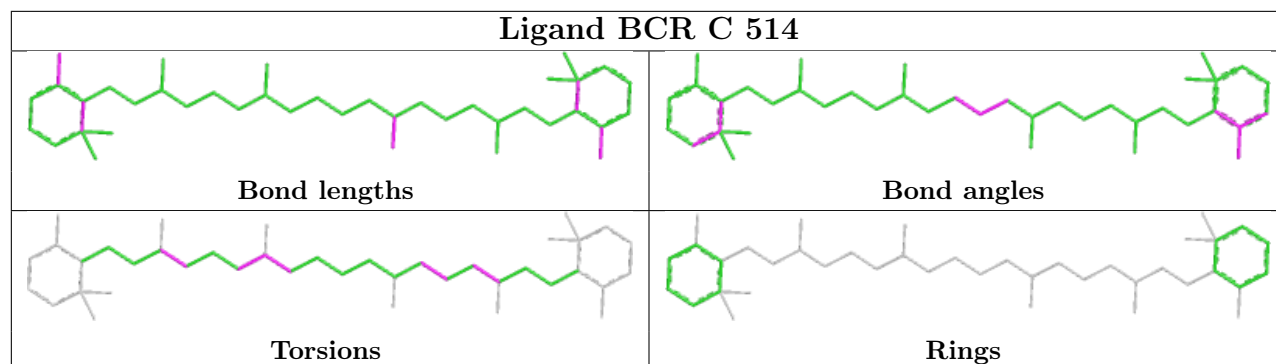
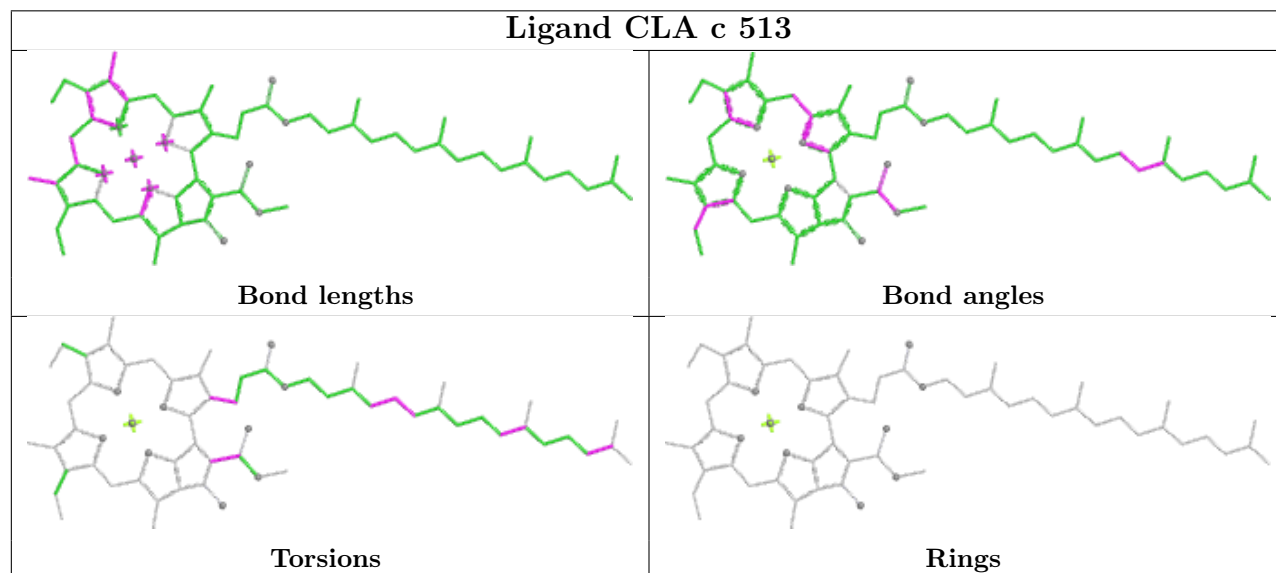
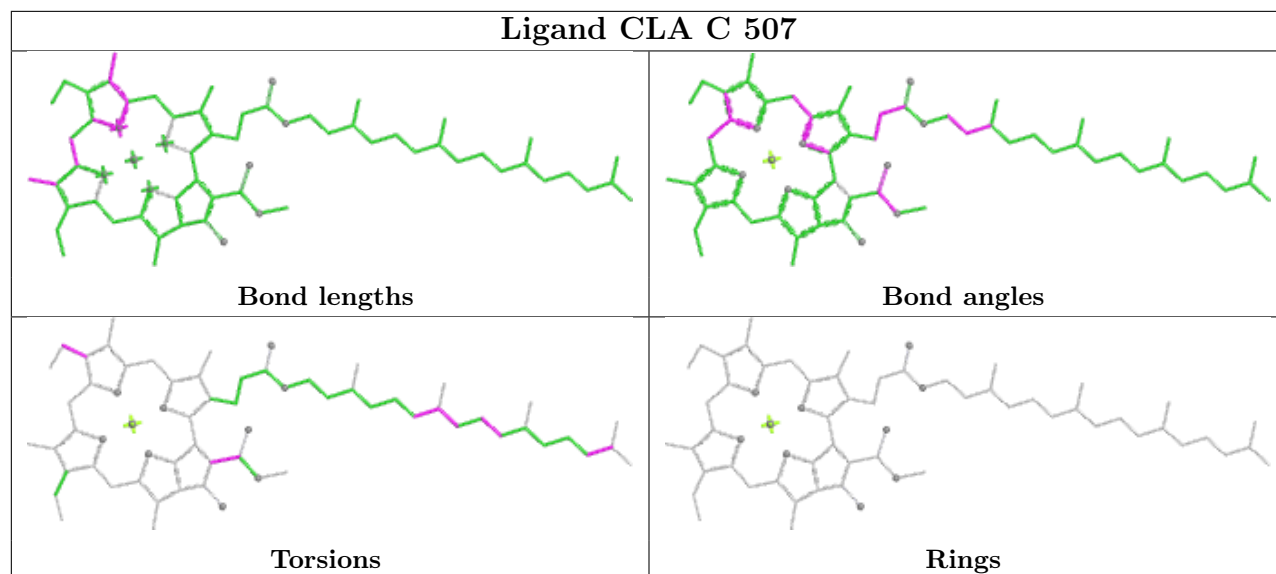
Ligand LHG d 406

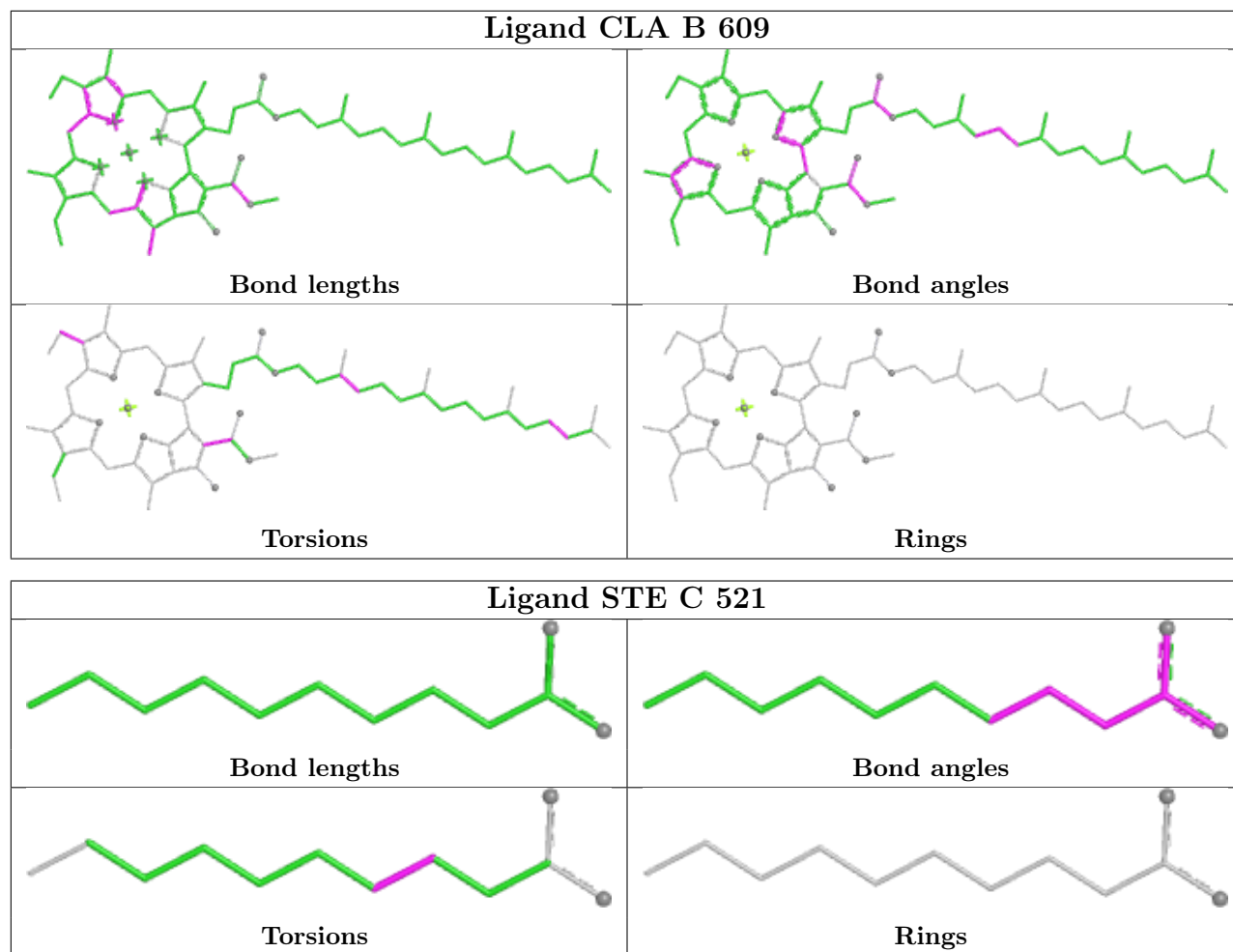


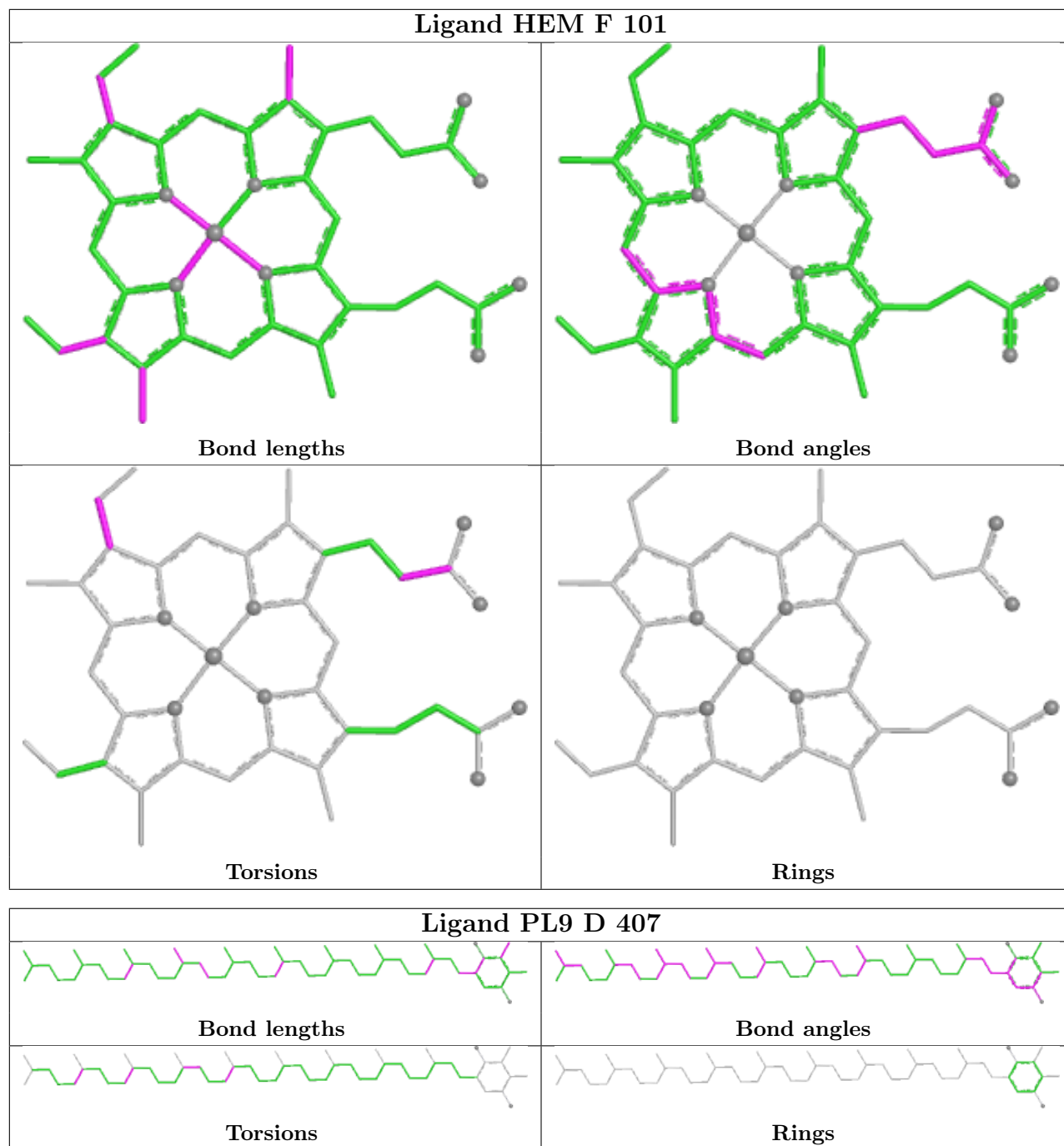
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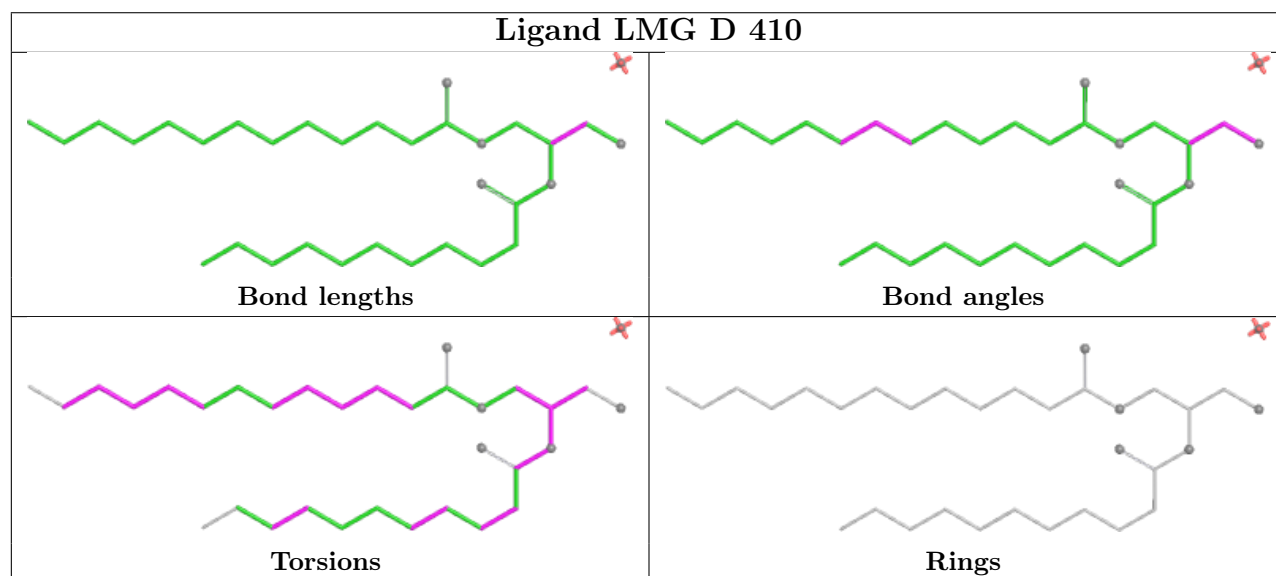
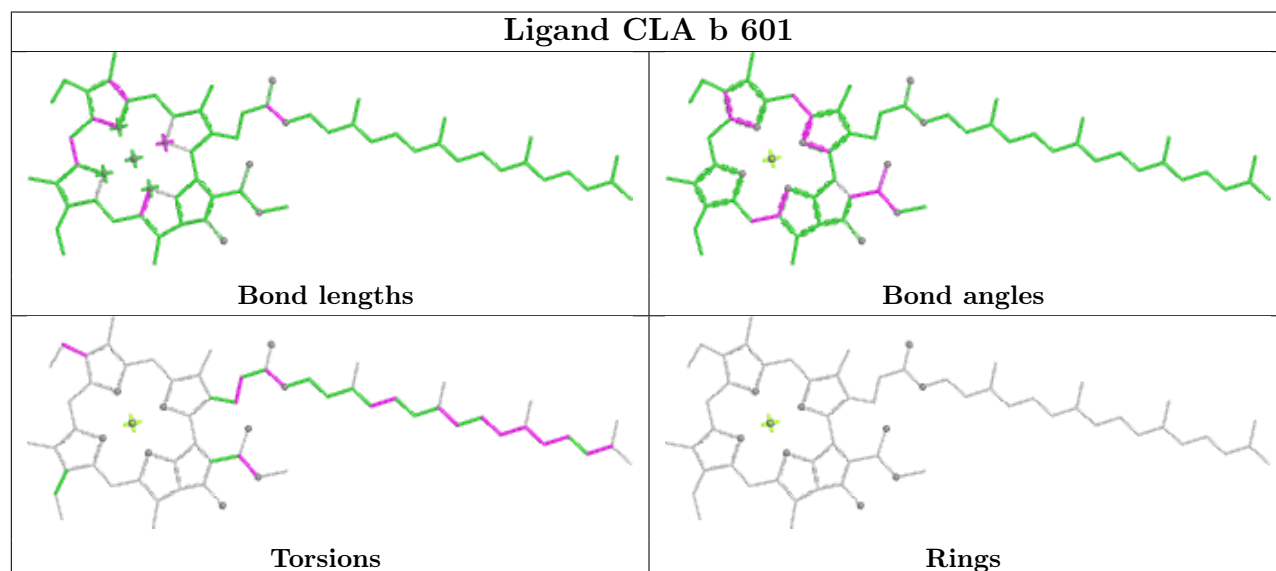
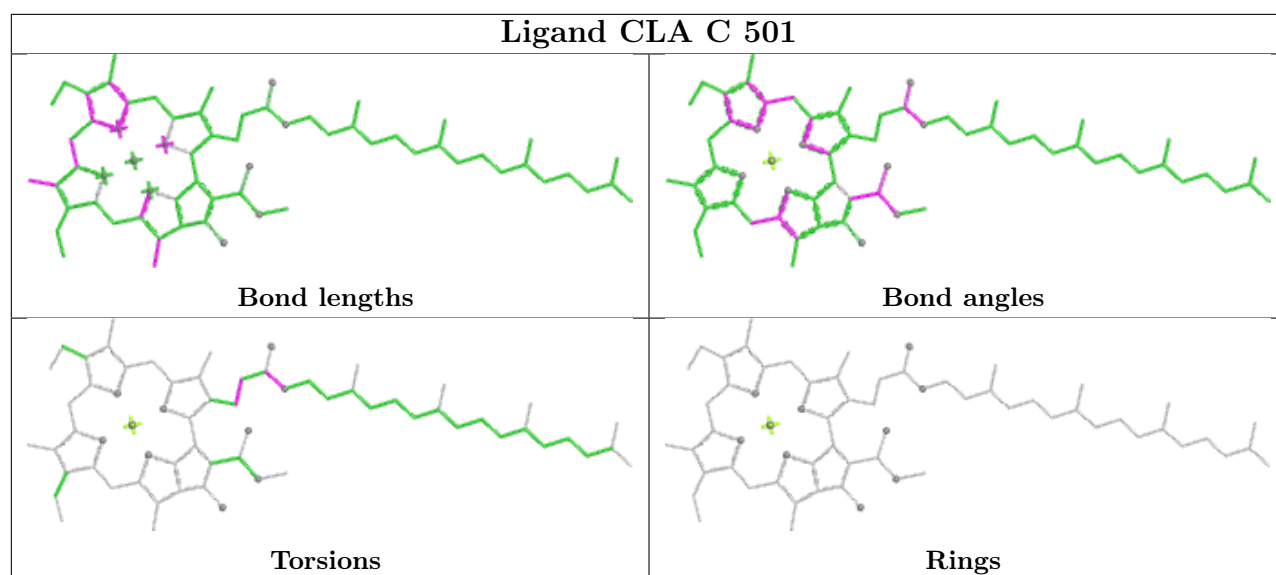


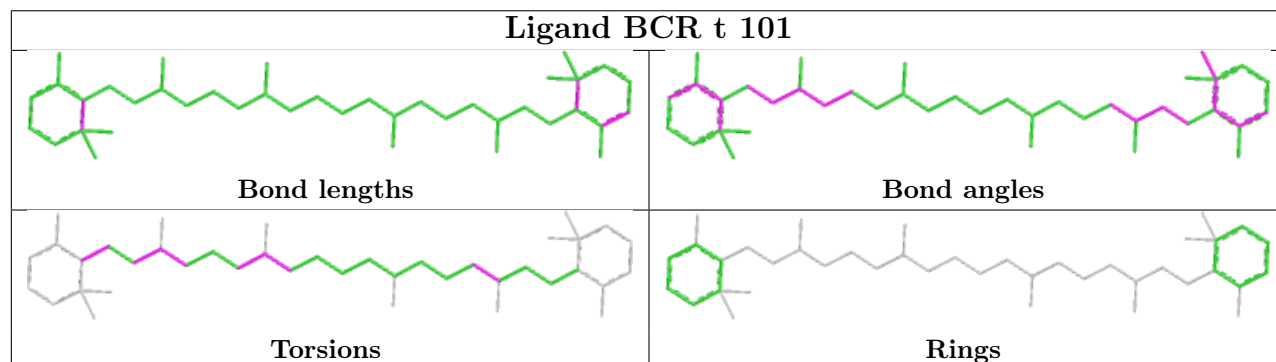
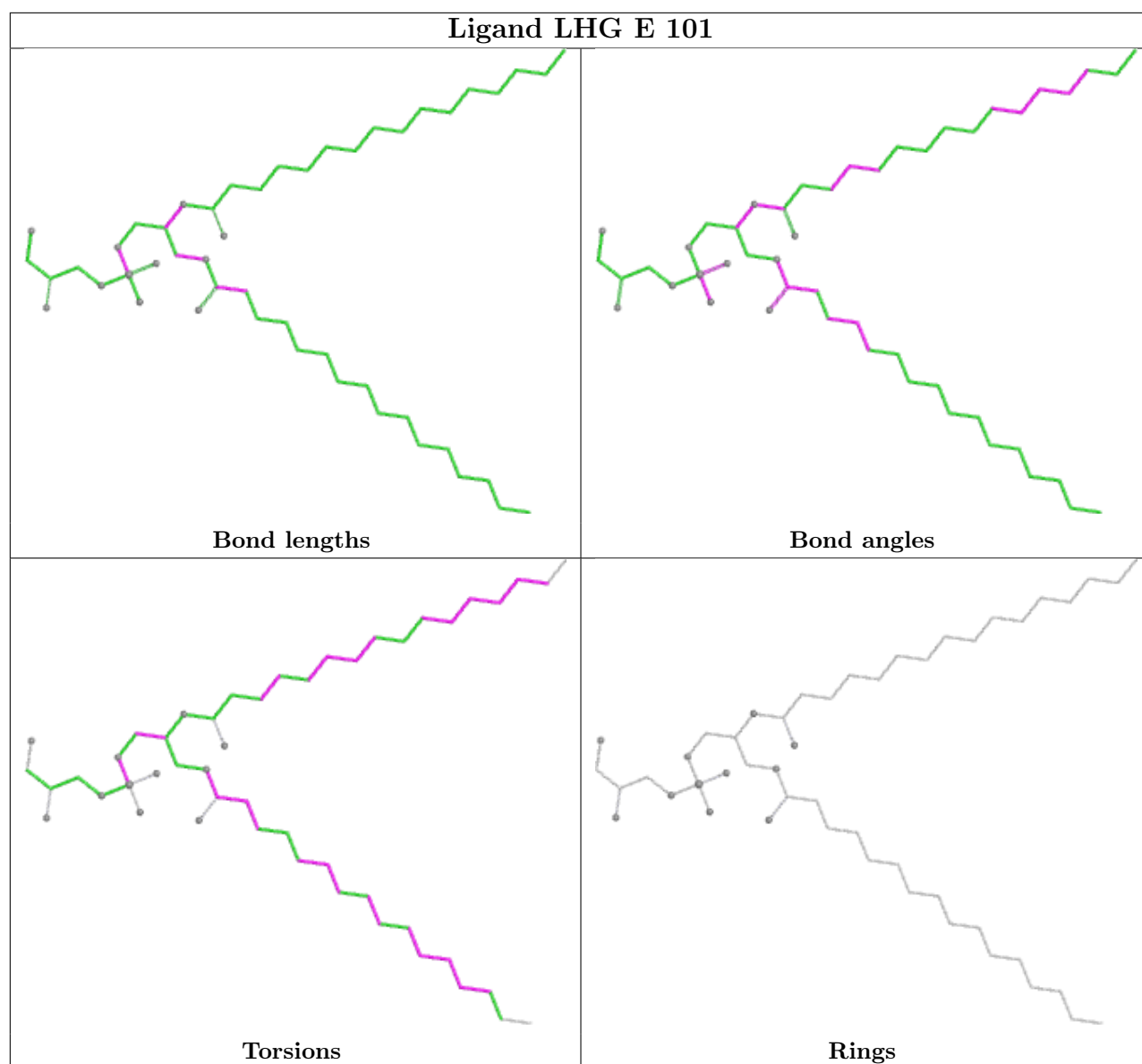


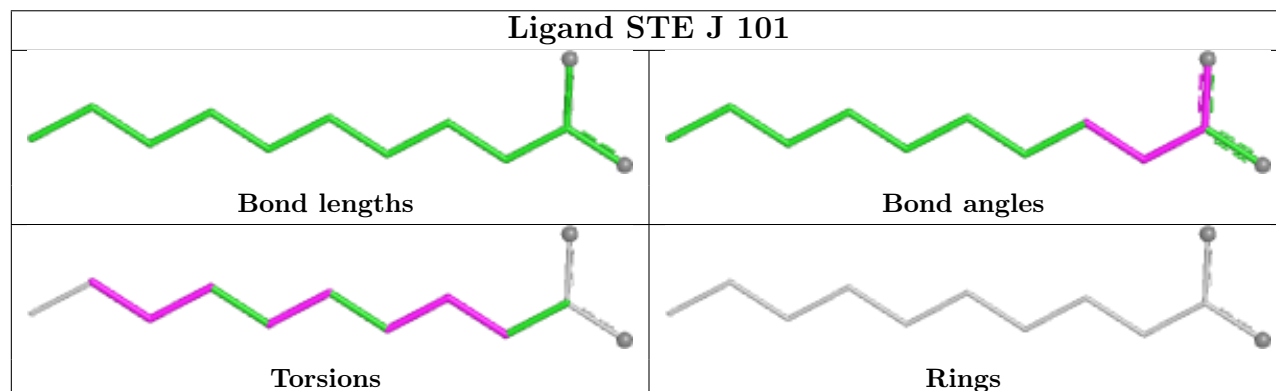
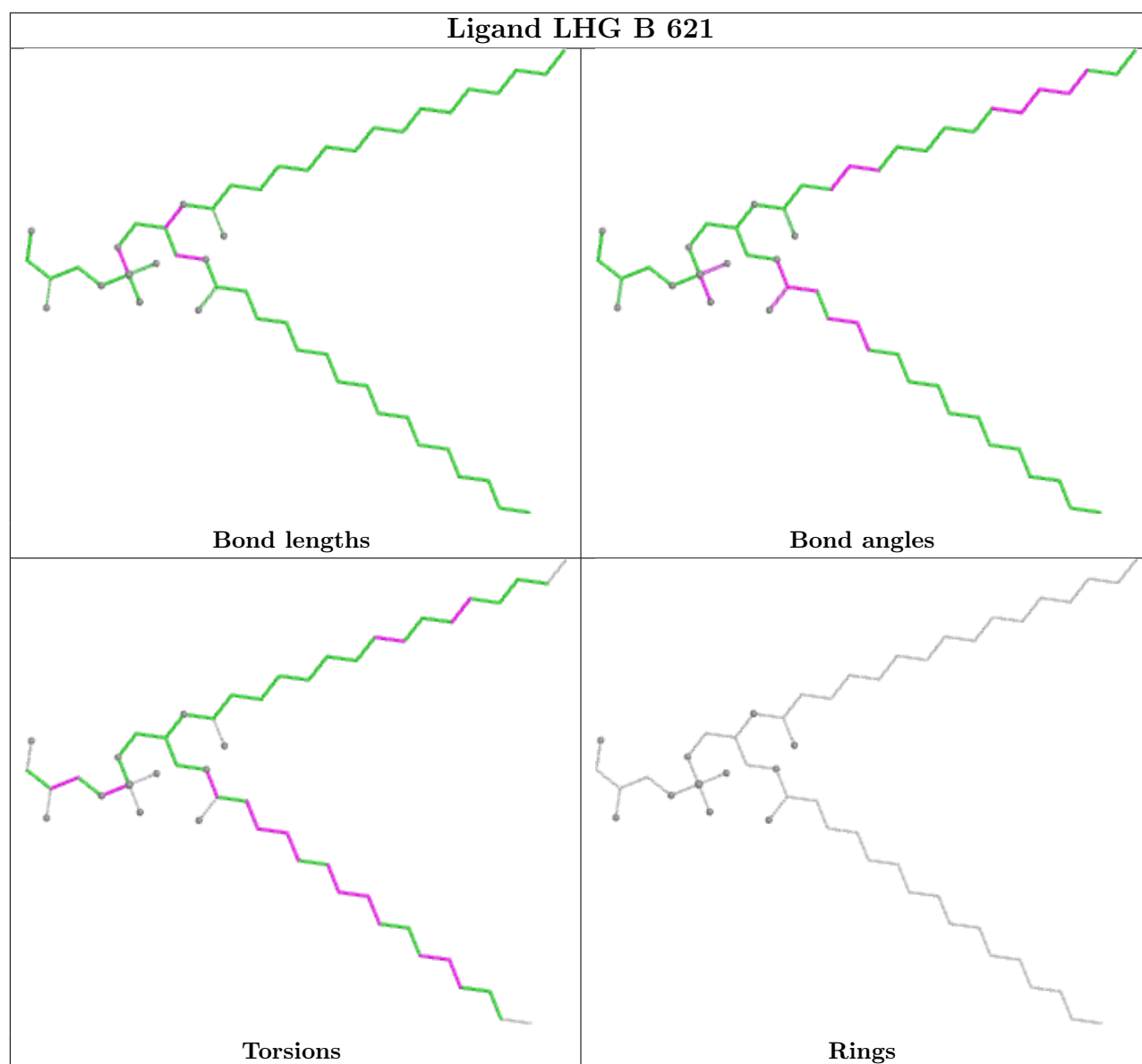


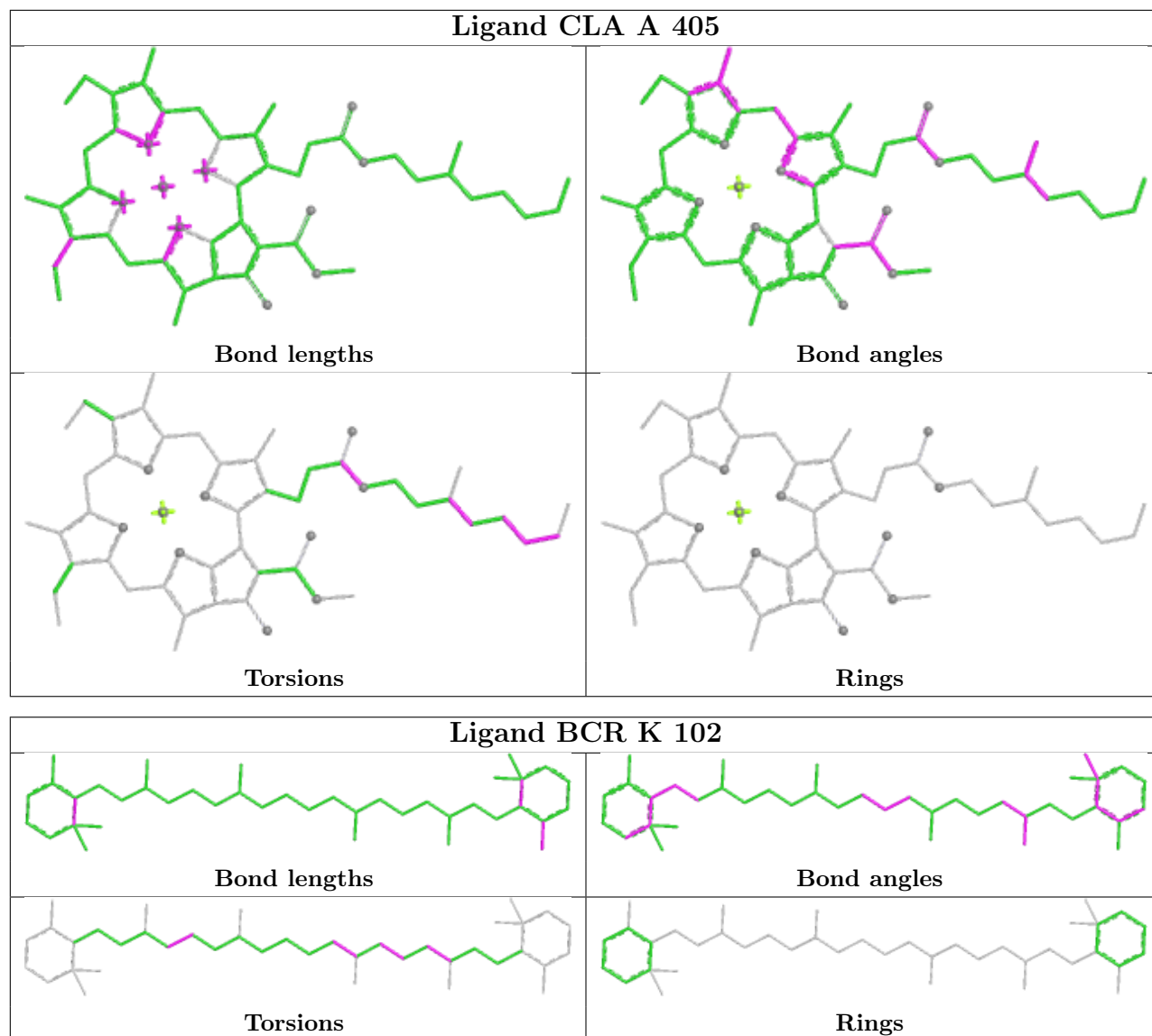




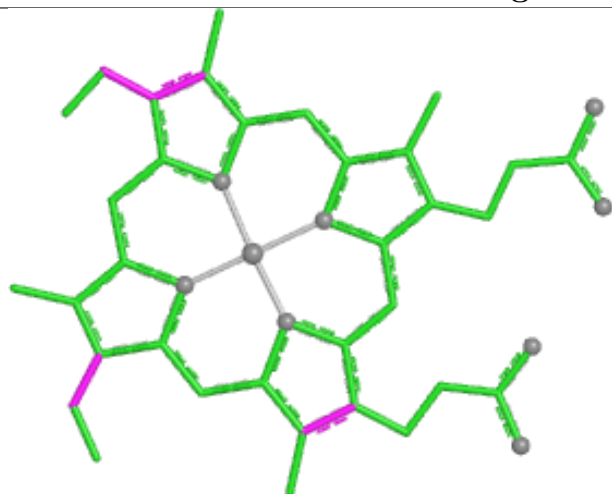




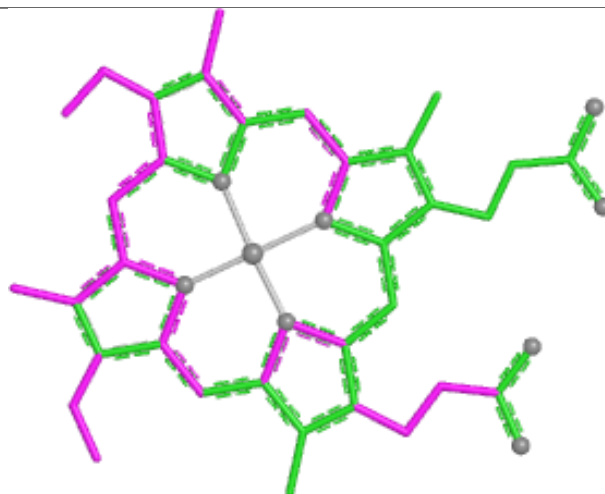




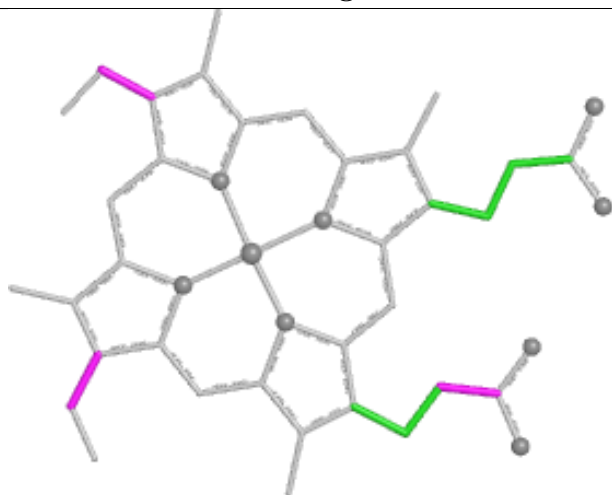
Ligand HEC V 201



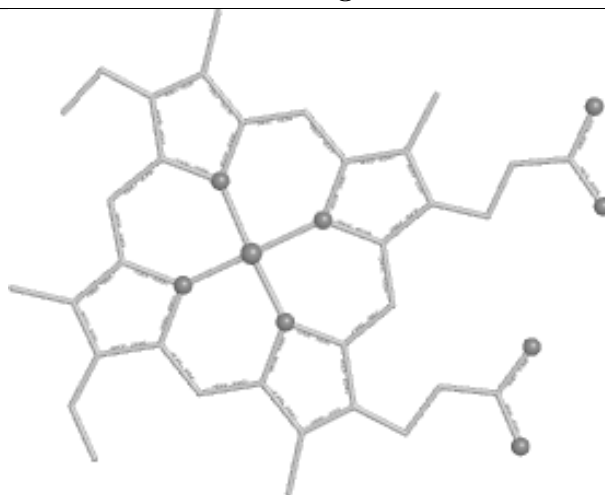
Bond lengths



Bond angles

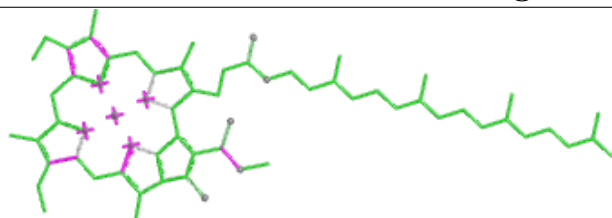


Torsions

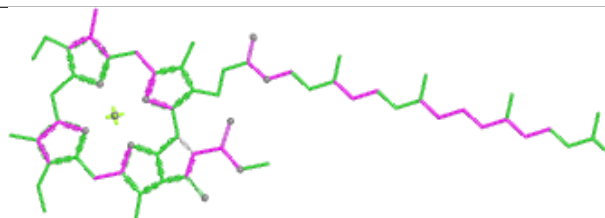


Rings

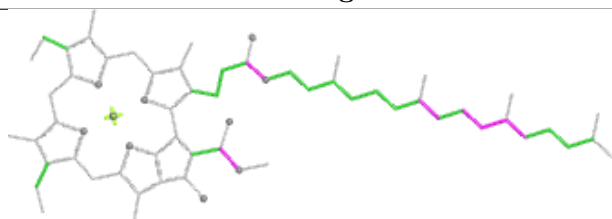
Ligand CLA B 604



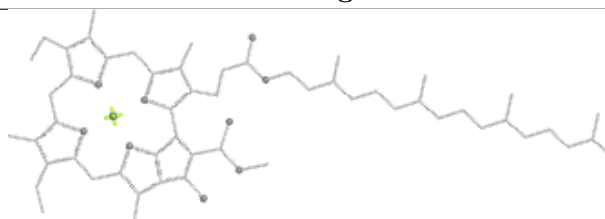
Bond lengths



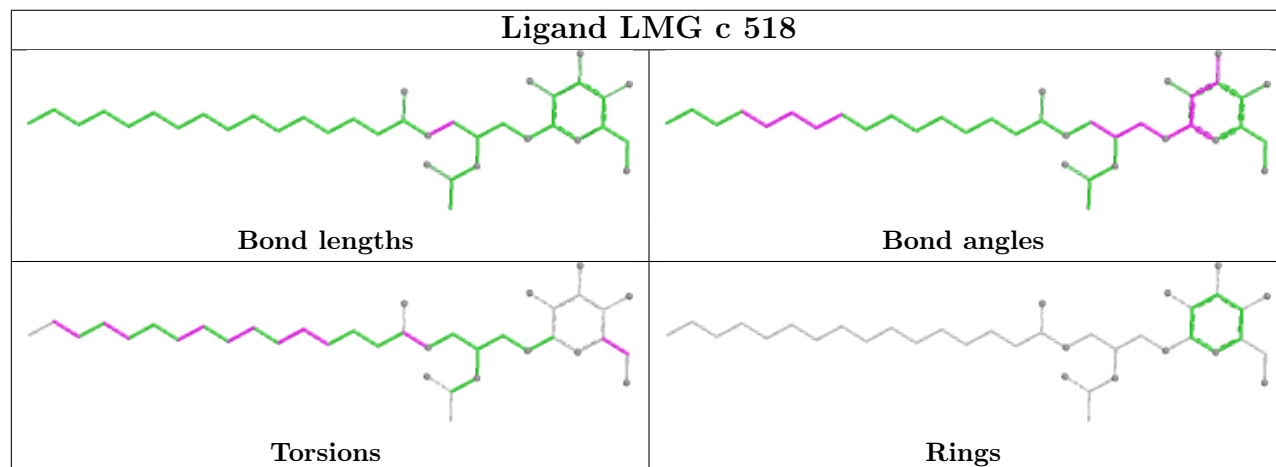
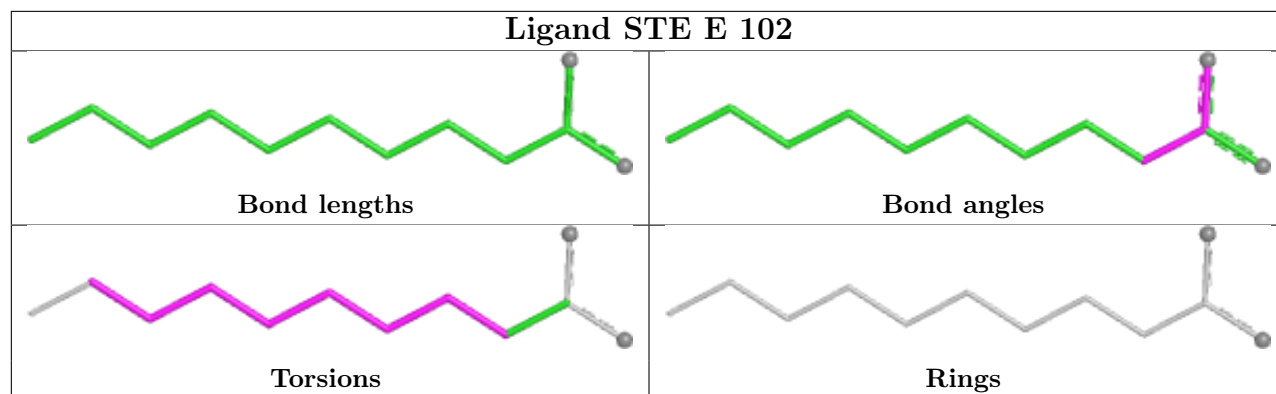
Bond angles

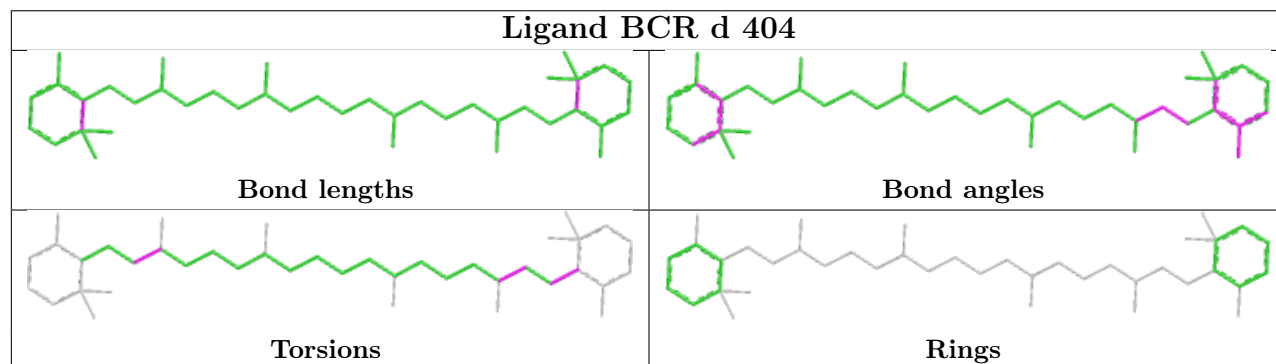
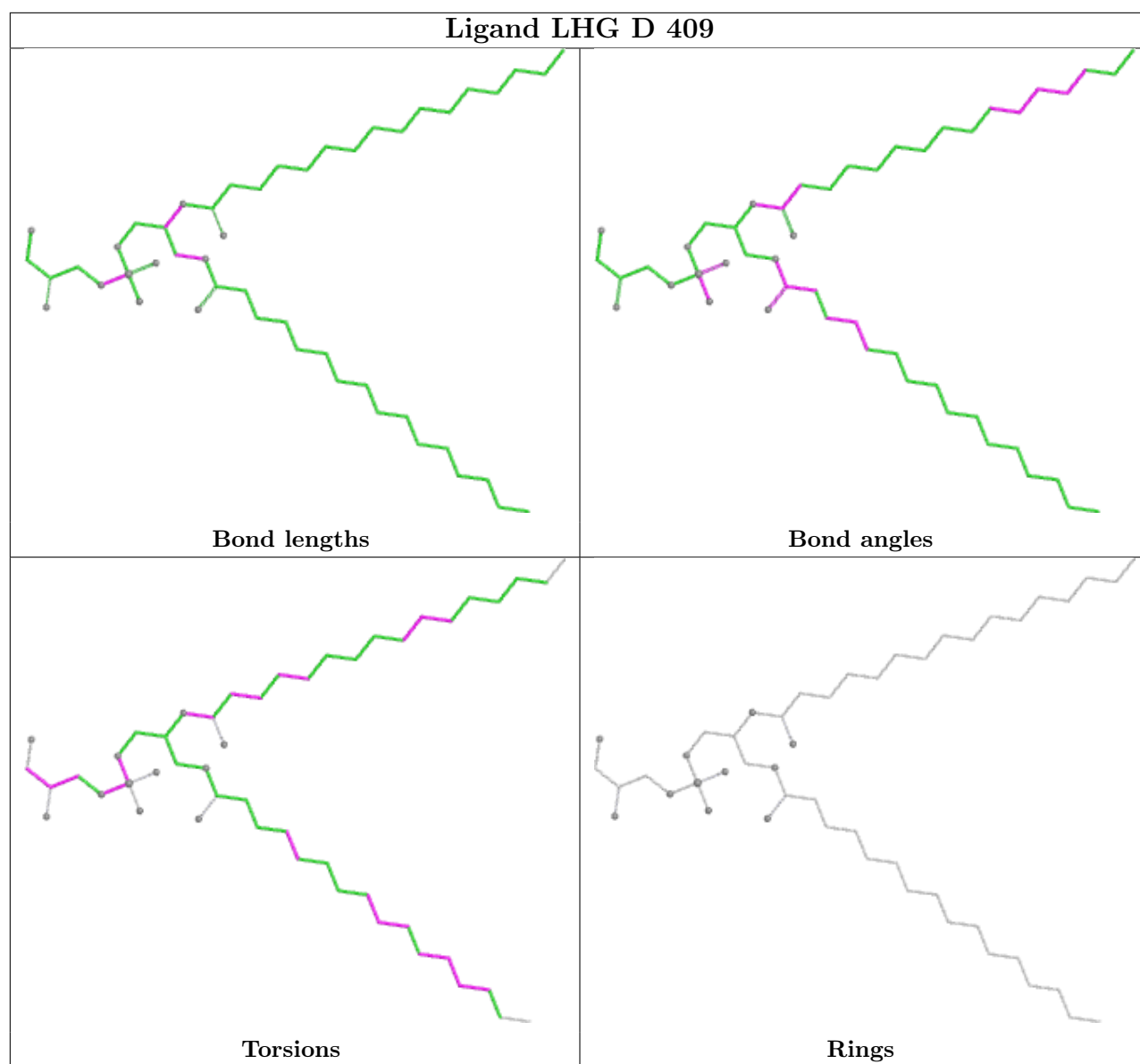


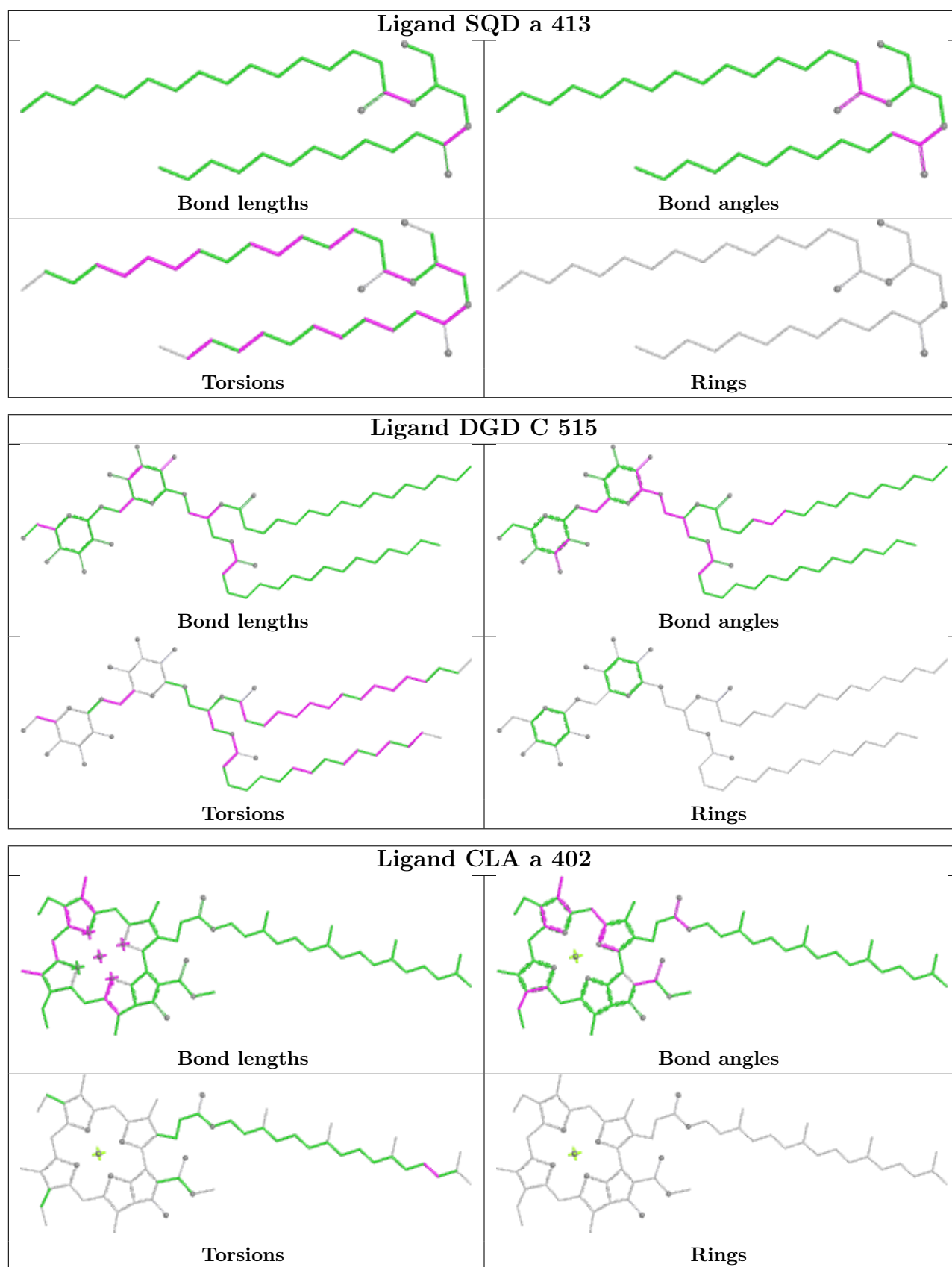
Torsions

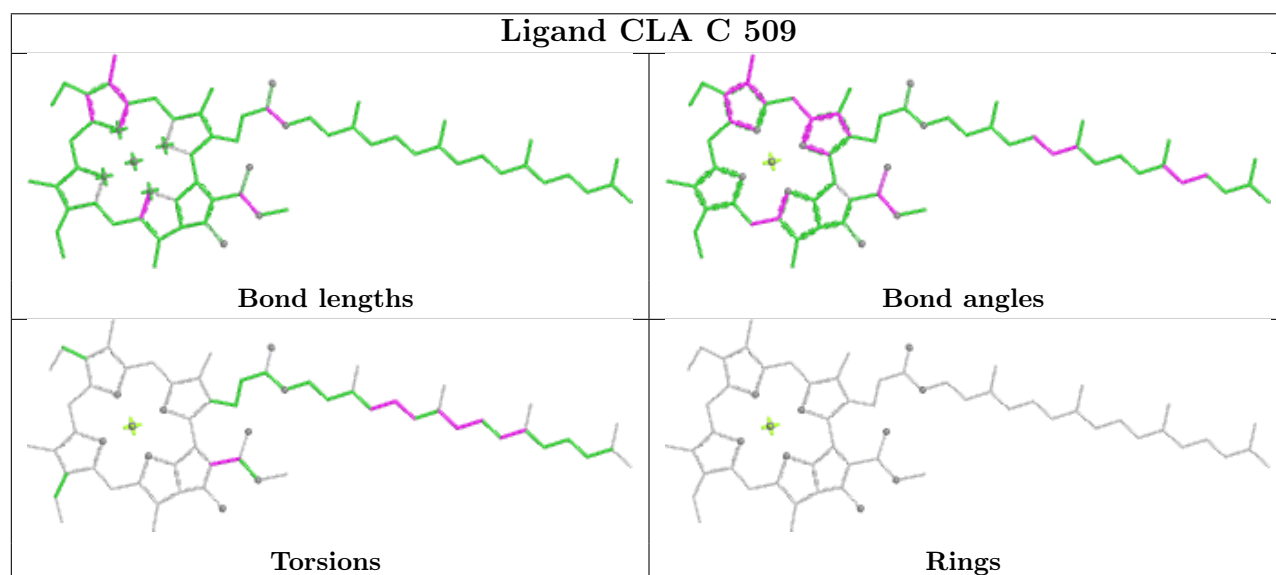
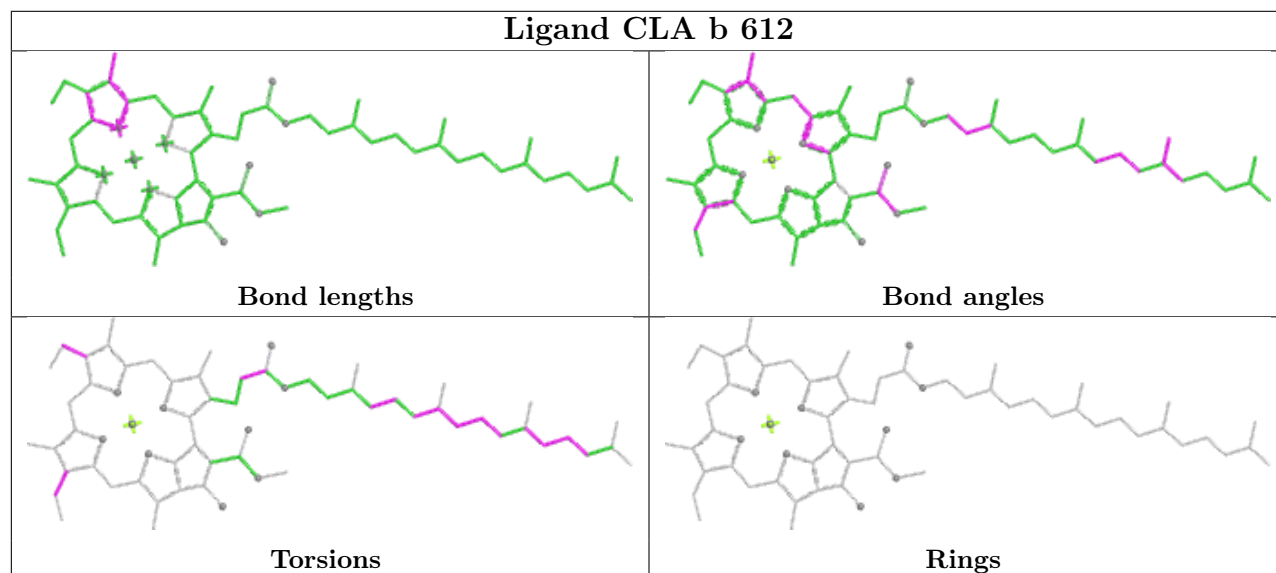
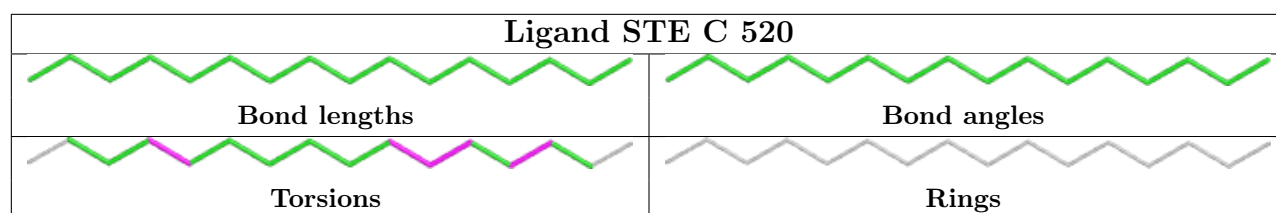


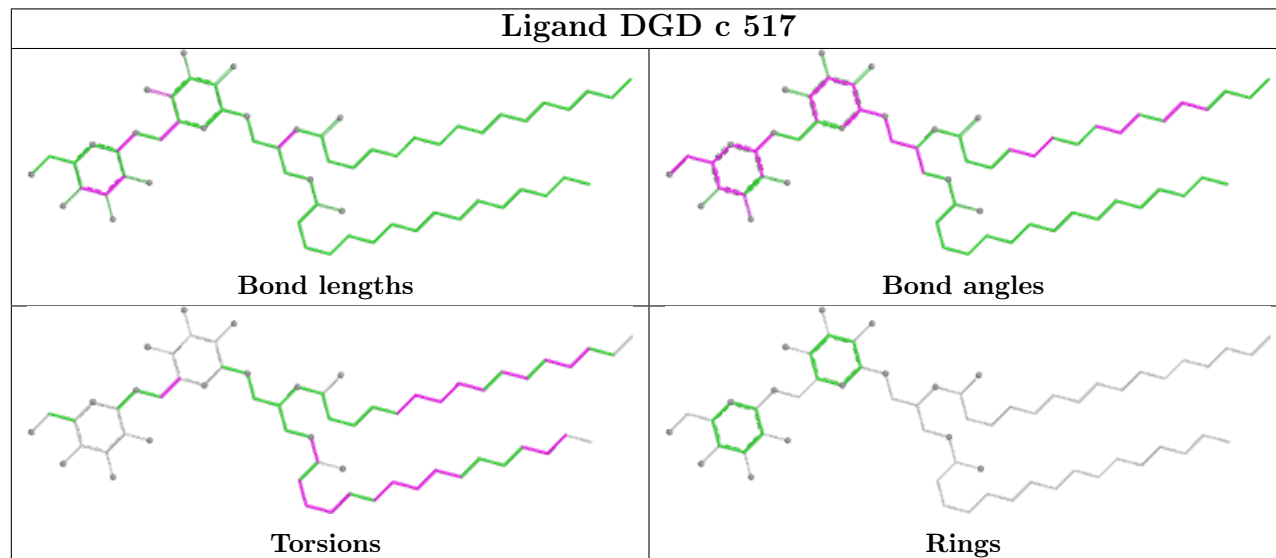
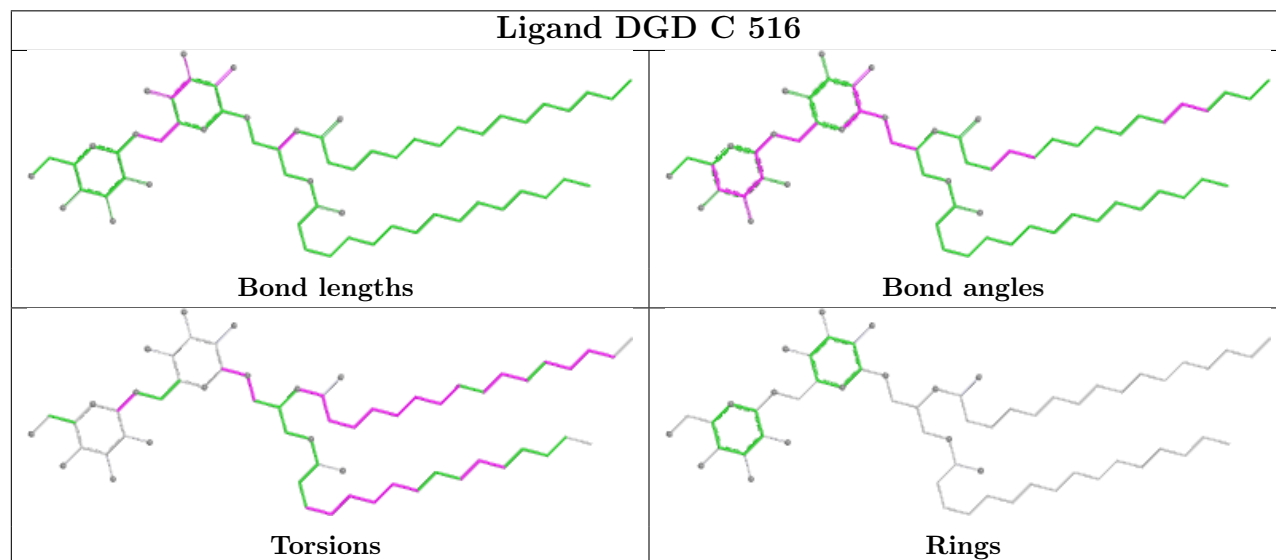
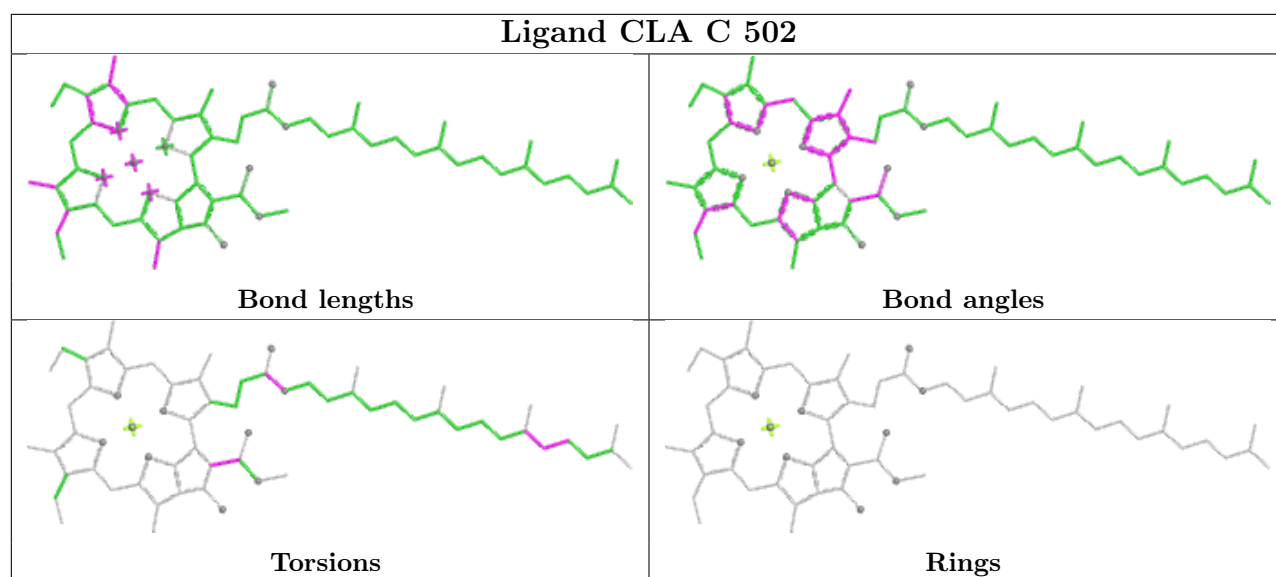
Rings

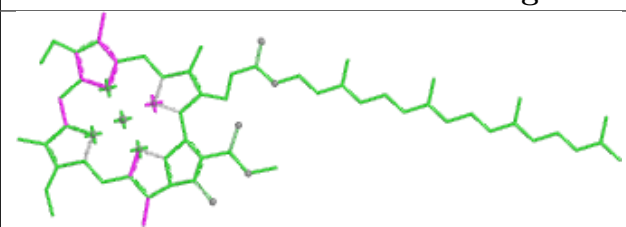
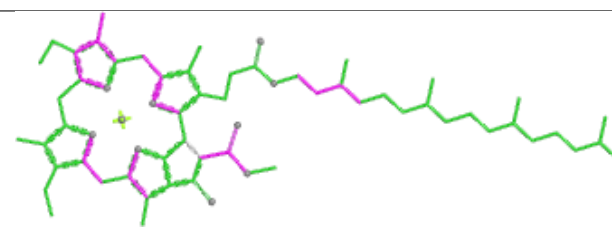
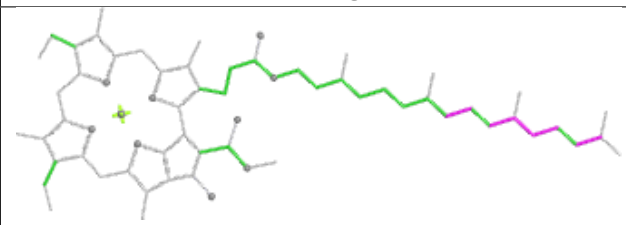
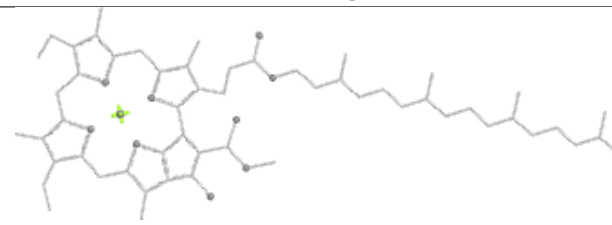


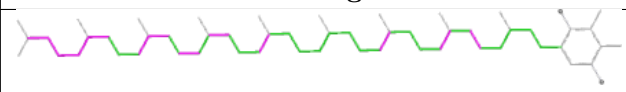
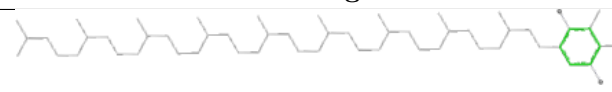


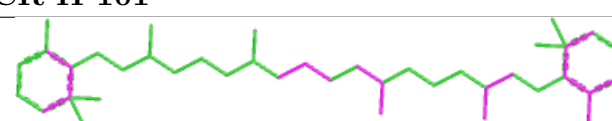
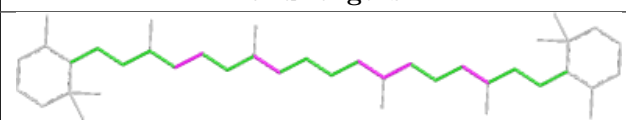
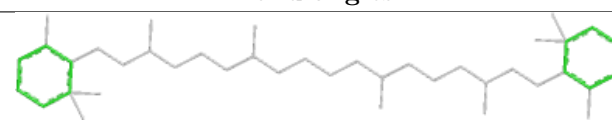




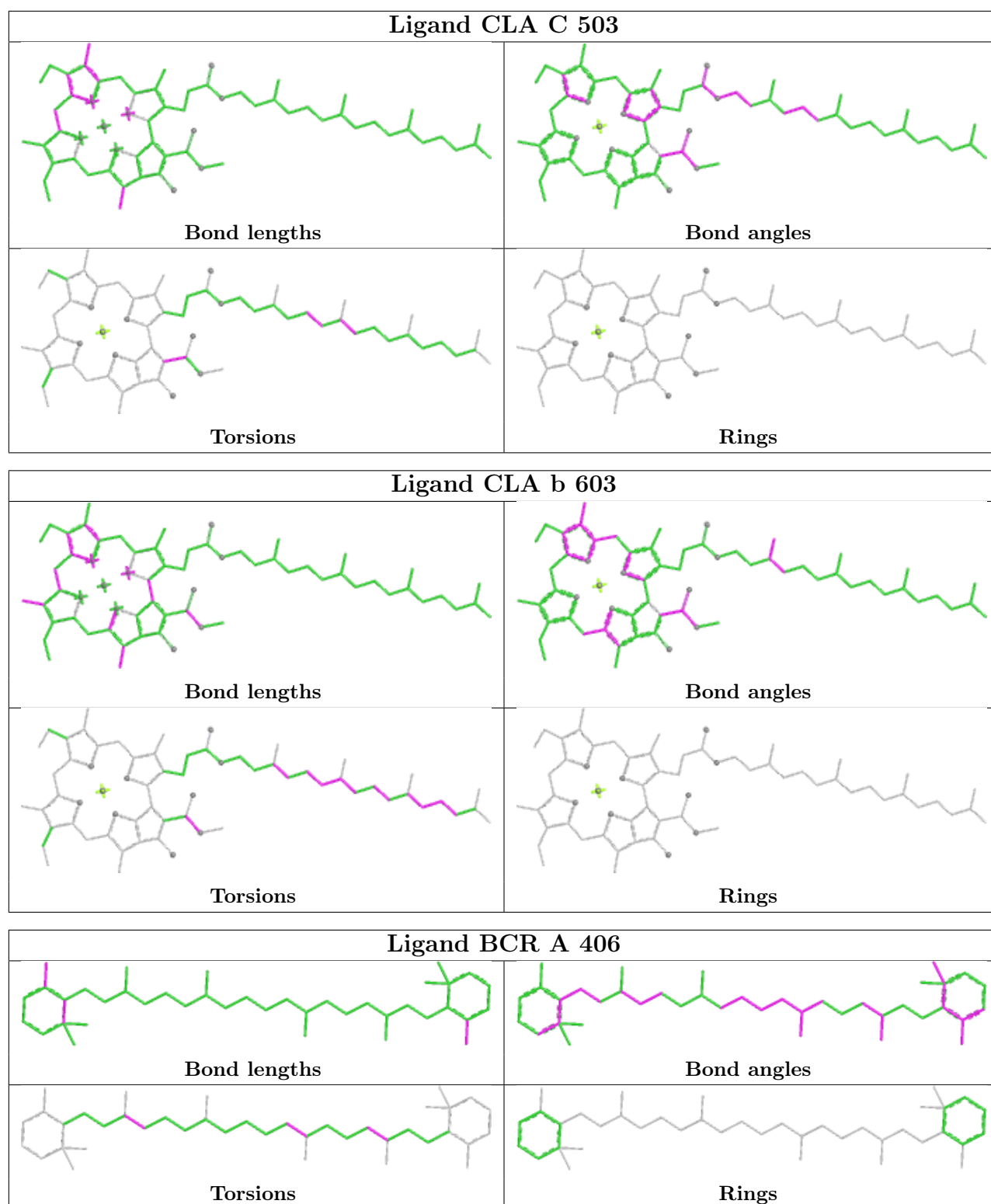


Ligand CLA B 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

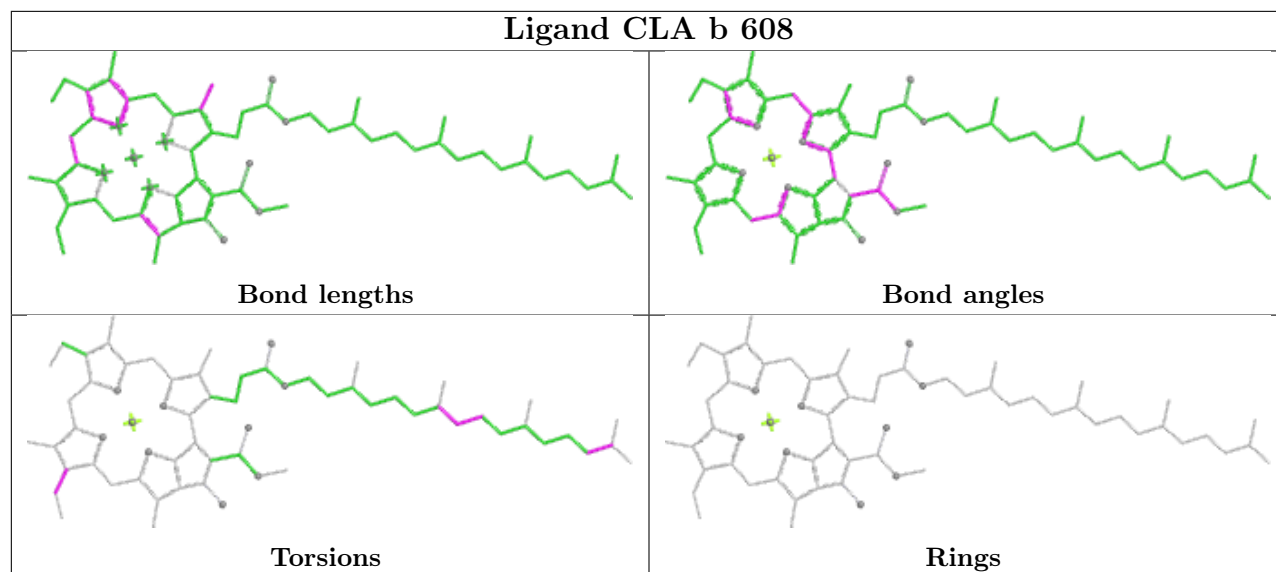
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

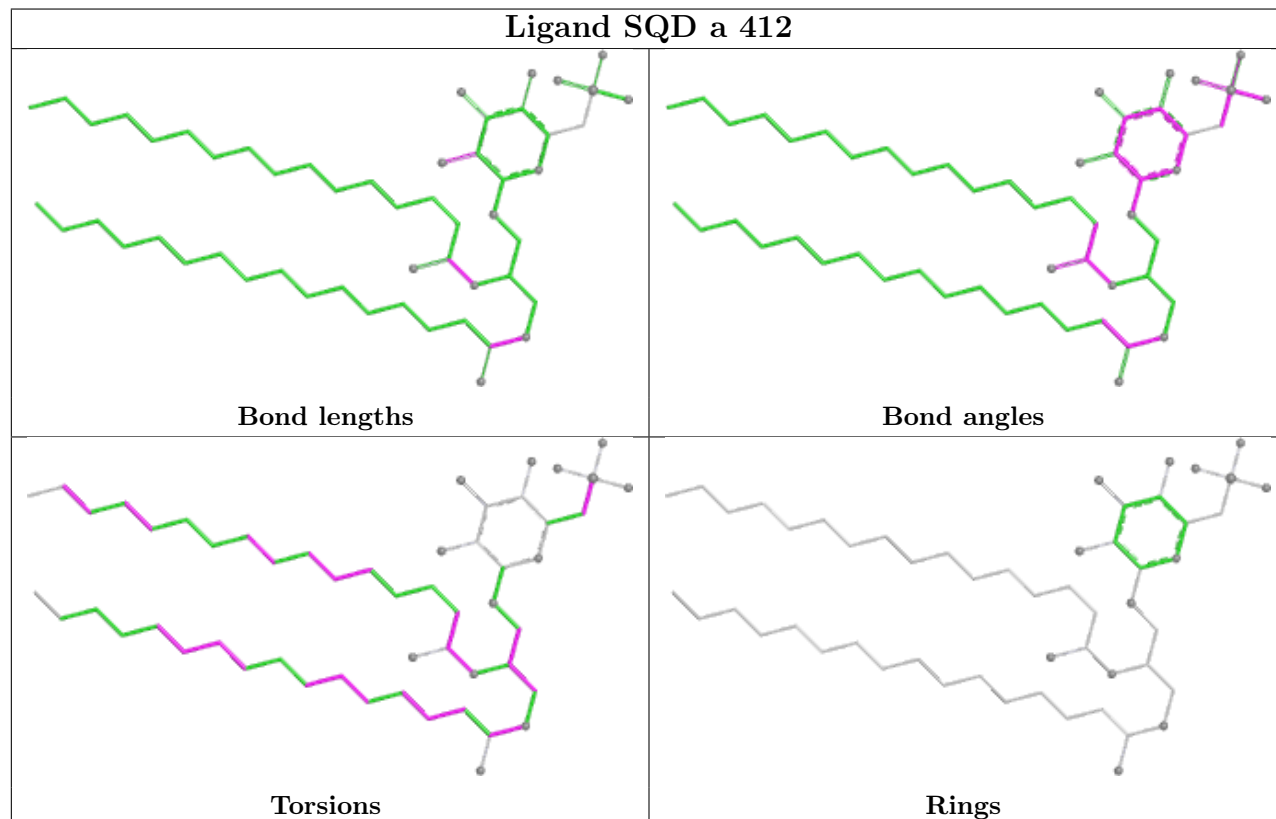
Ligand STE M 104	
	
Bond lengths	Bond angles
	
Torsions	Rings



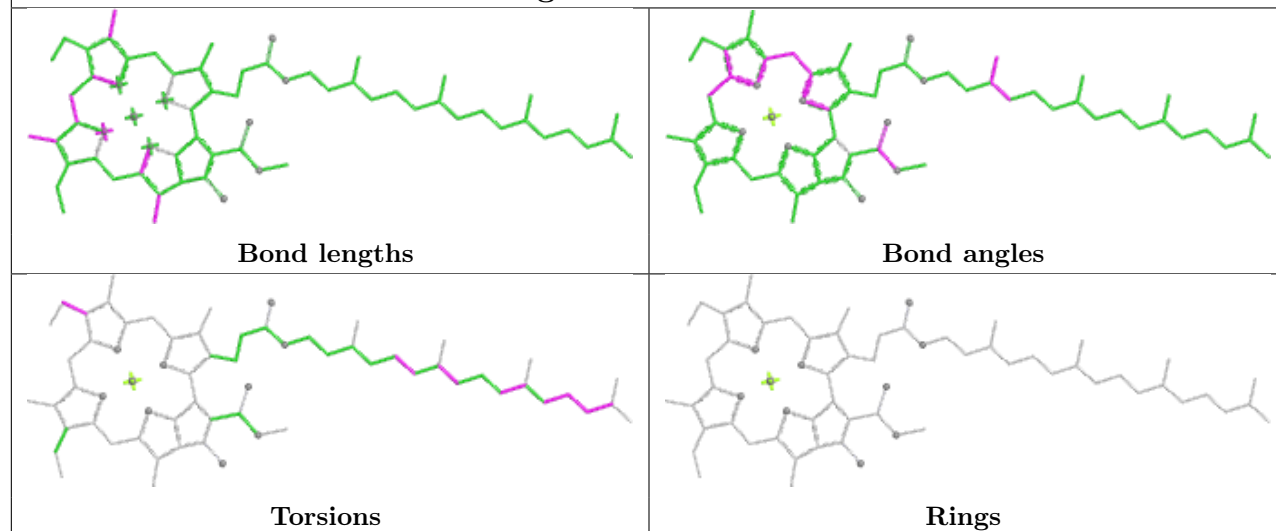
Ligand CLA b 608



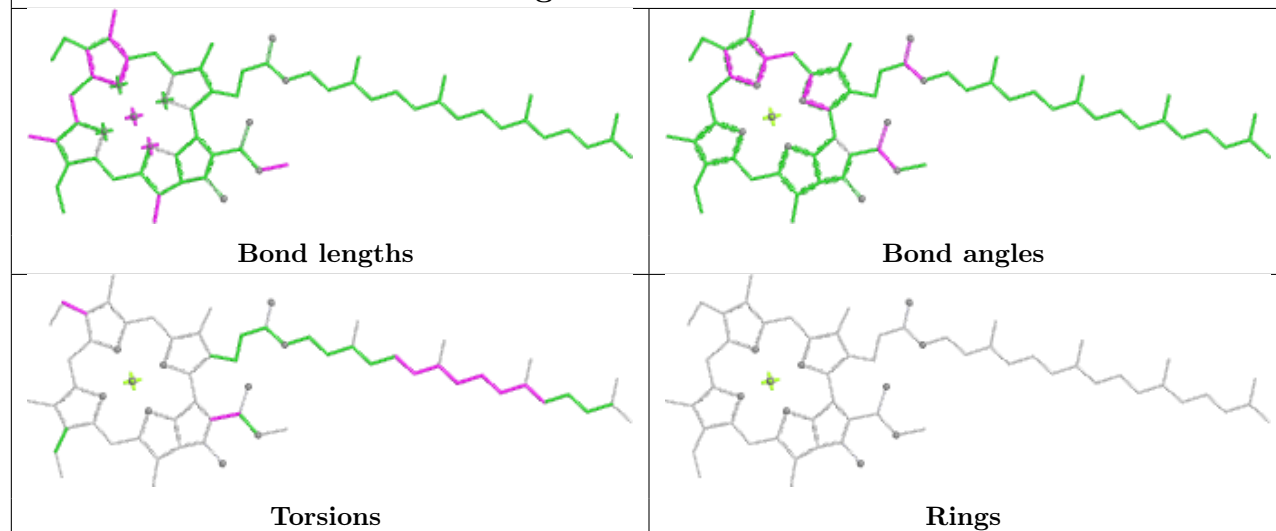
Ligand SQD a 412



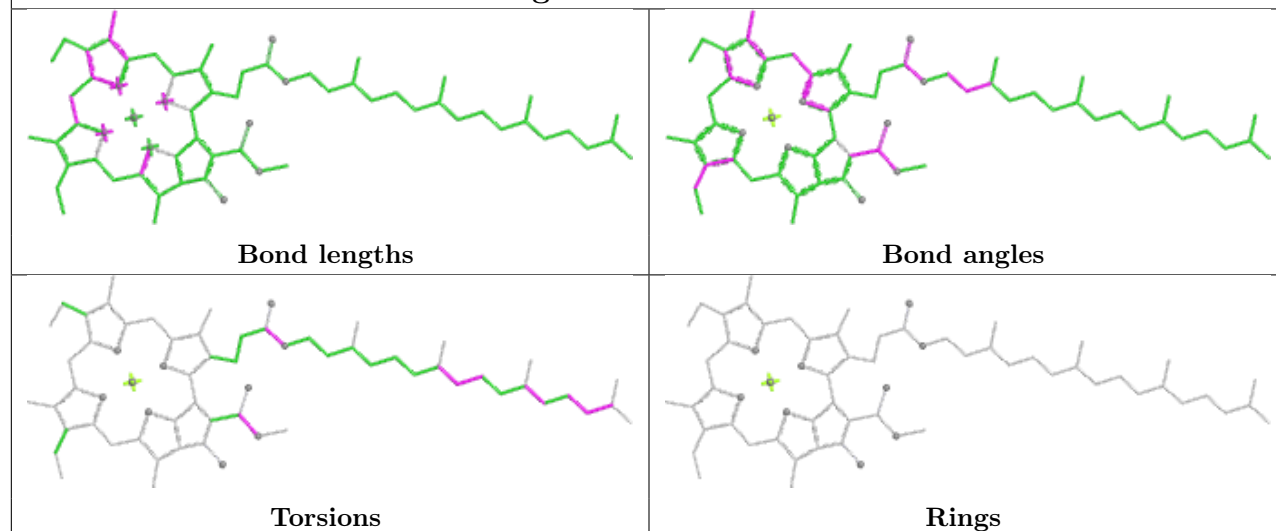
Ligand CLA c 503



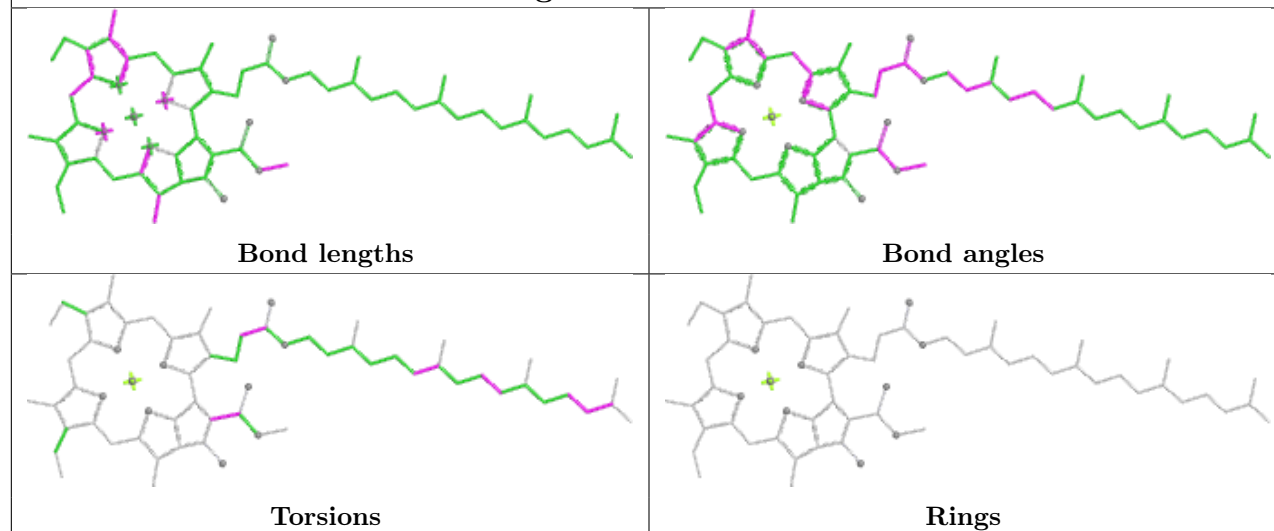
Ligand CLA b 607



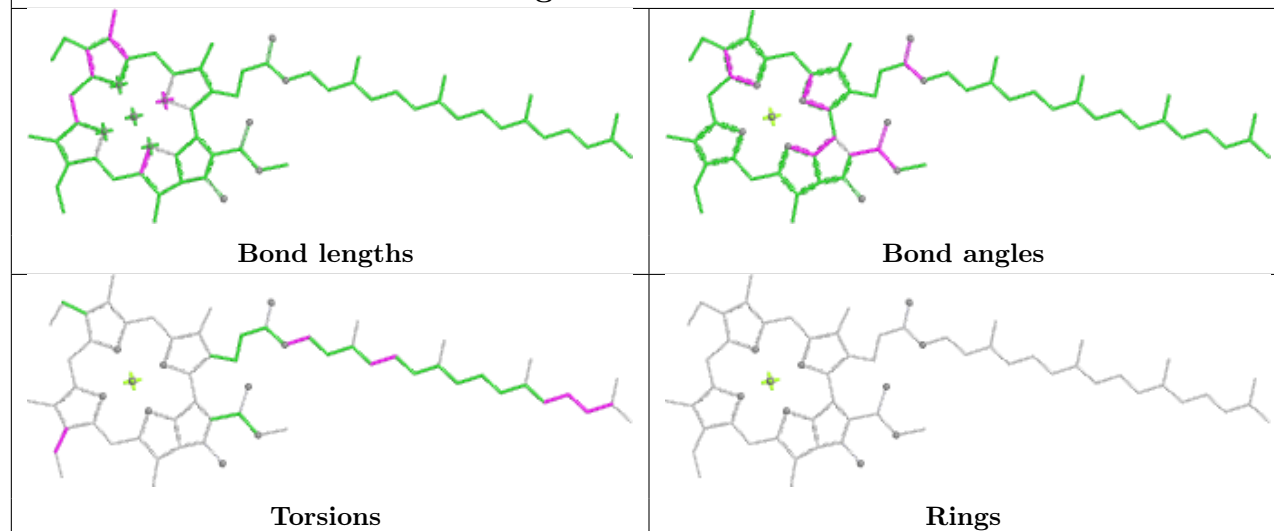
Ligand CLA C 511



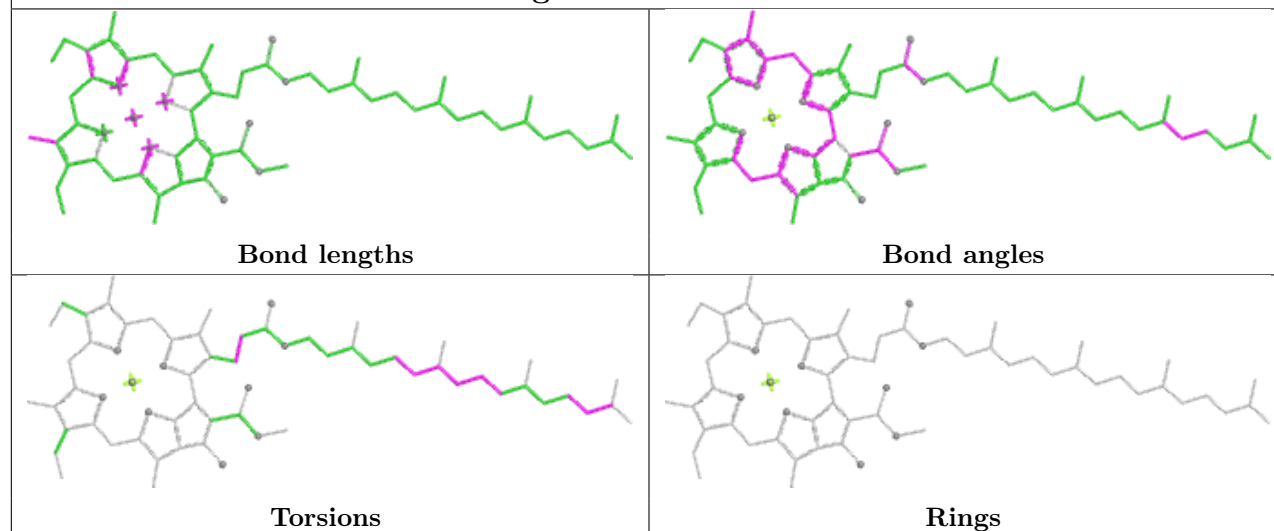
Ligand CLA b 613



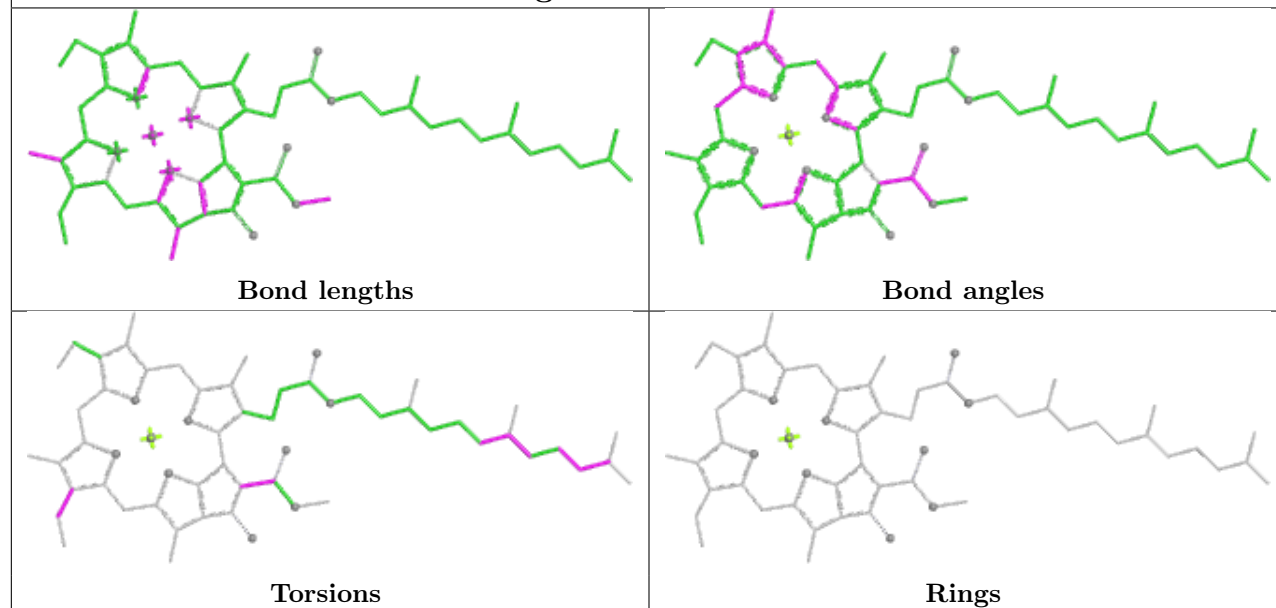
Ligand CLA d 402



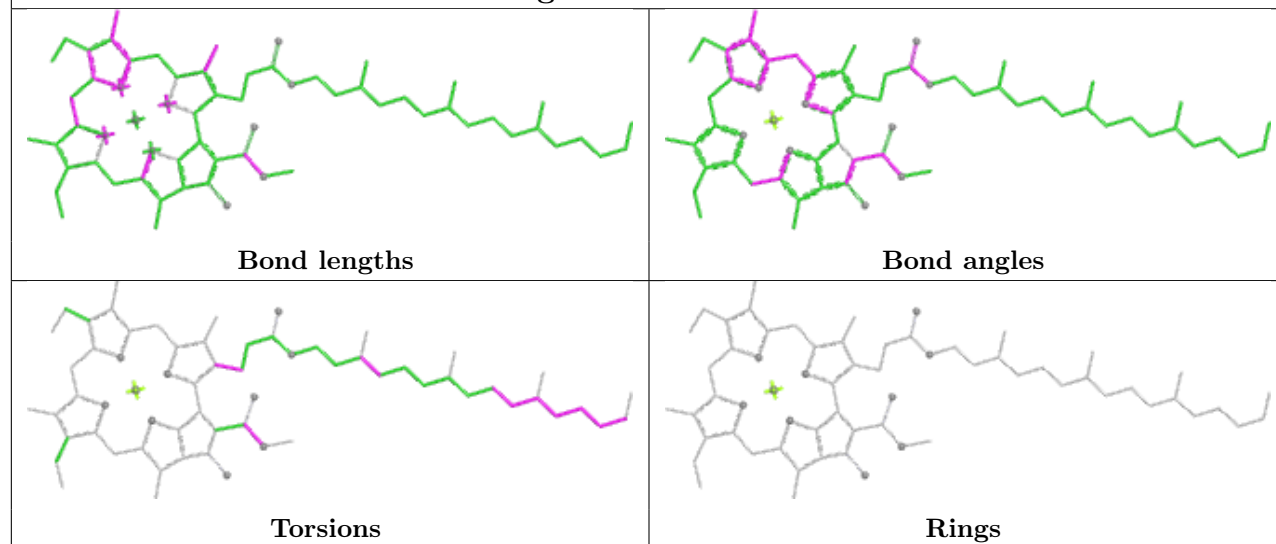
Ligand CLA B 603



Ligand CLA b 616

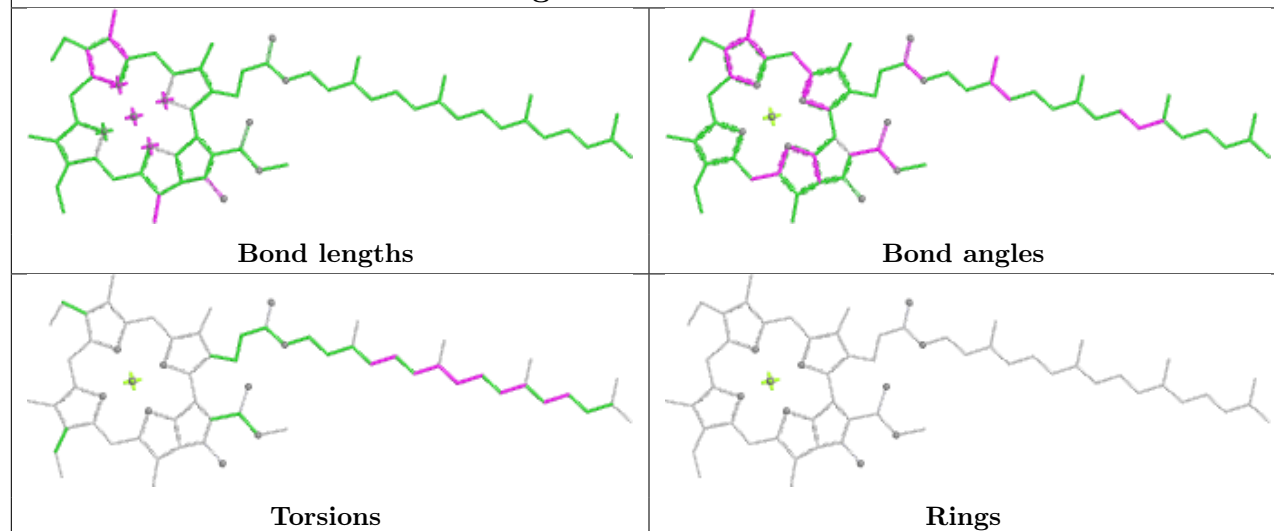
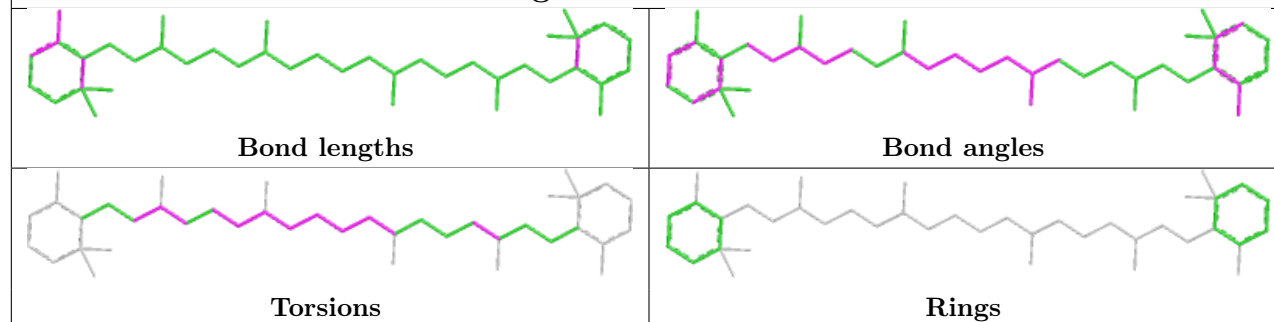
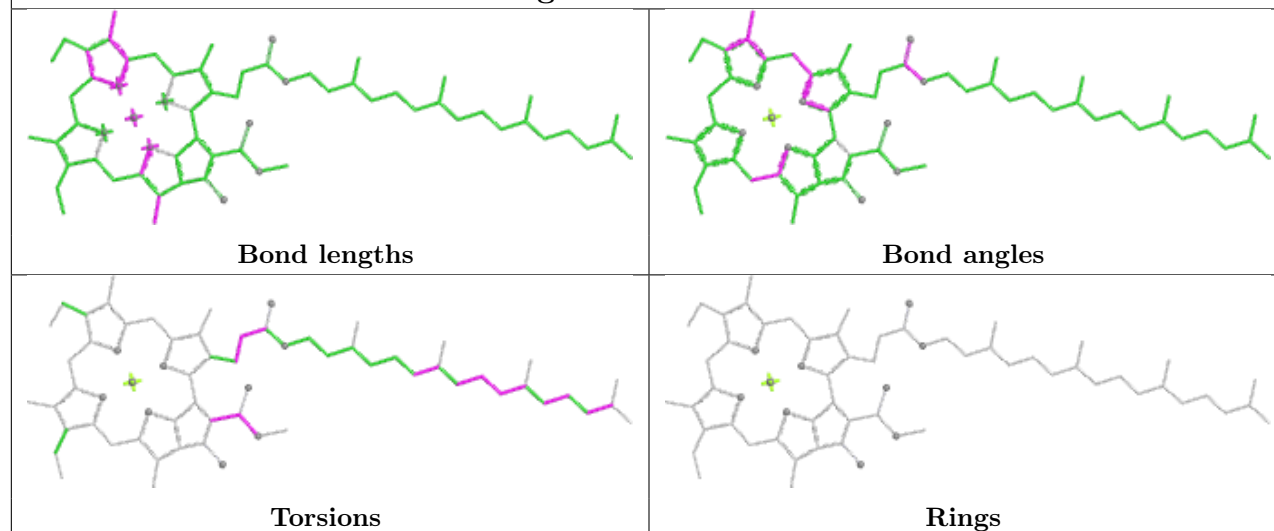


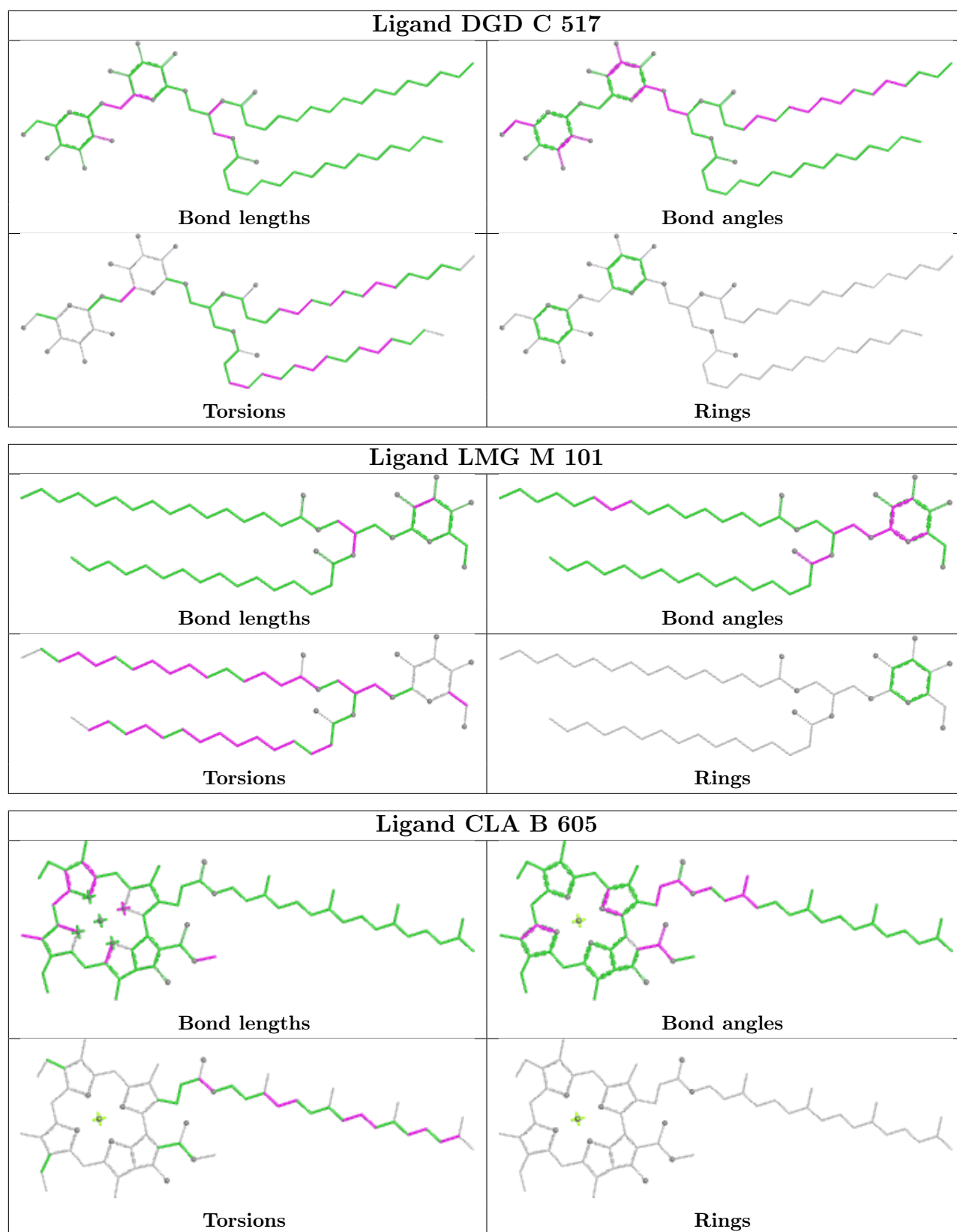
Ligand CLA c 508

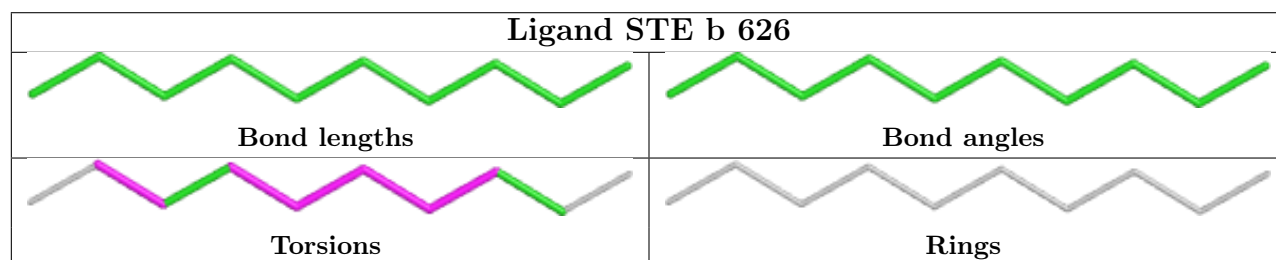
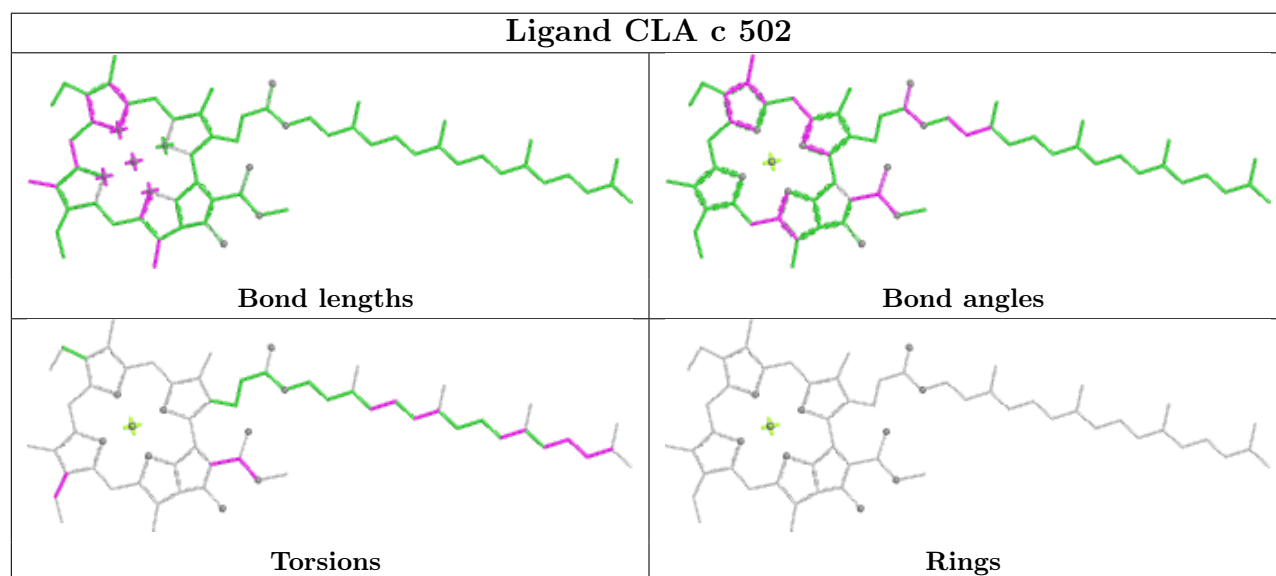
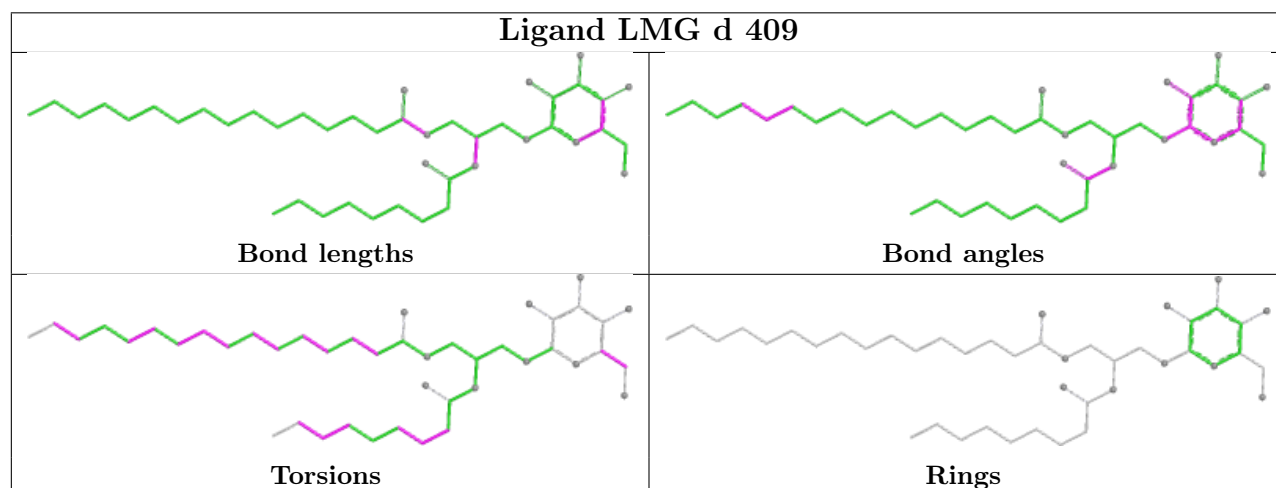
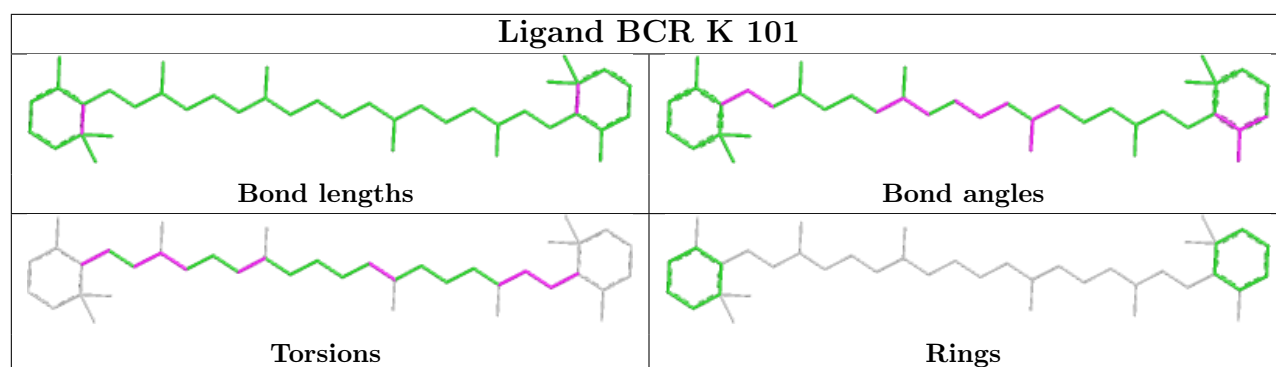


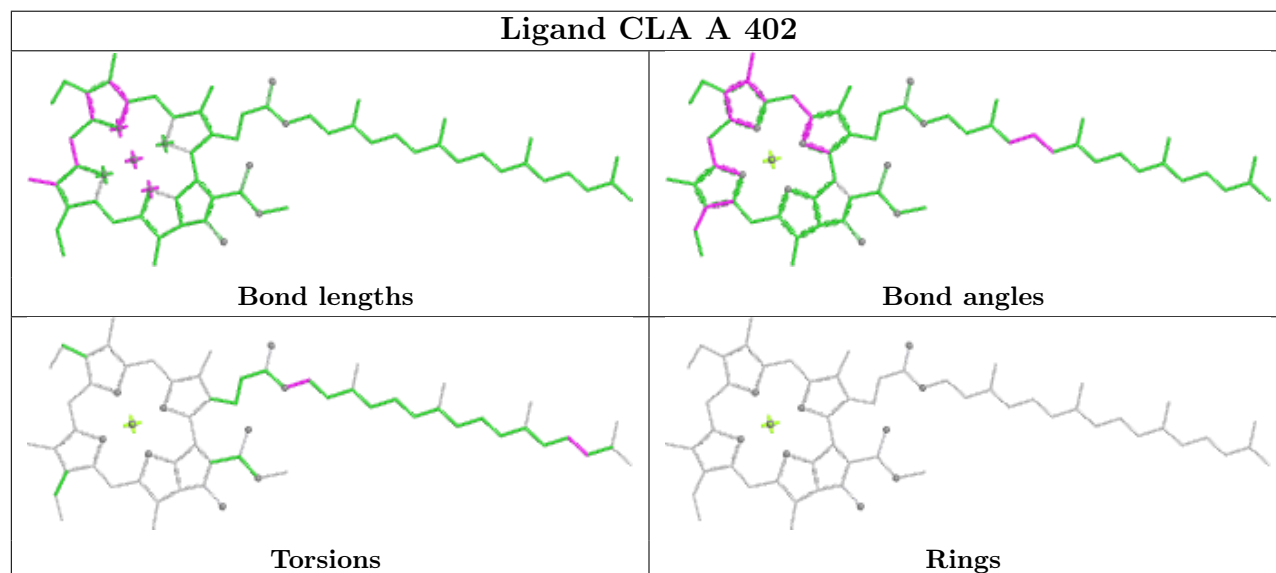
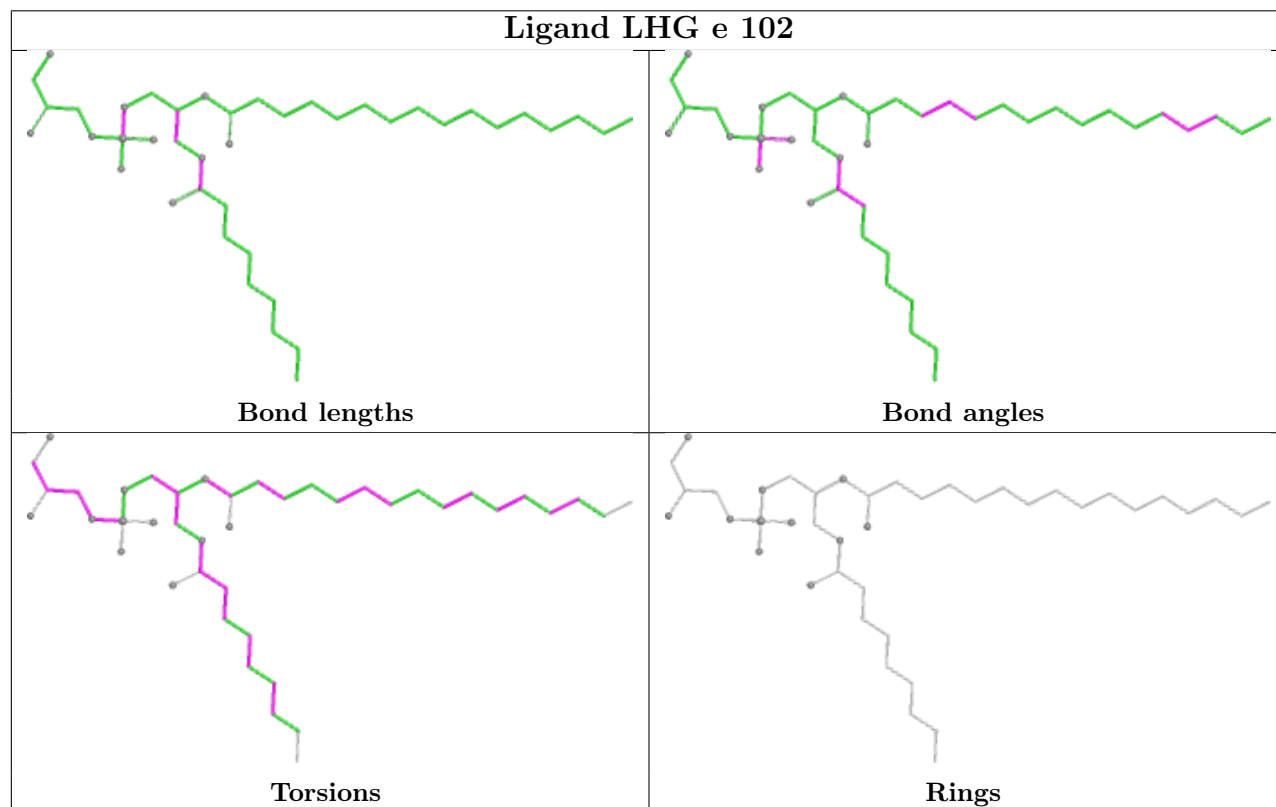
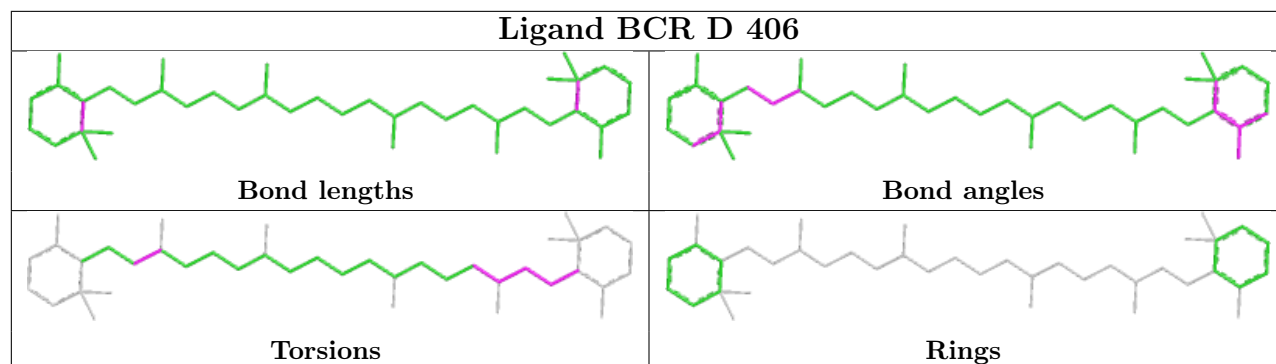
Ligand STE l 102

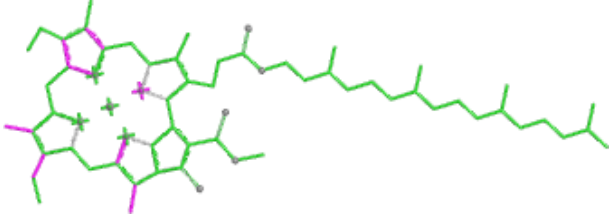
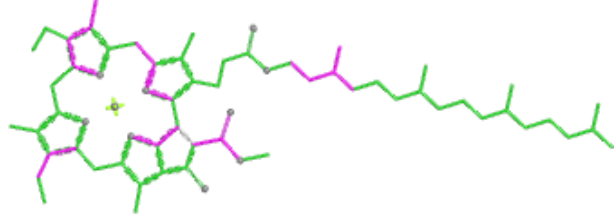
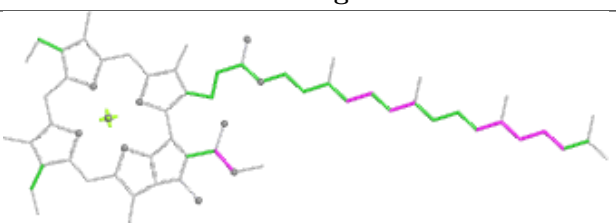
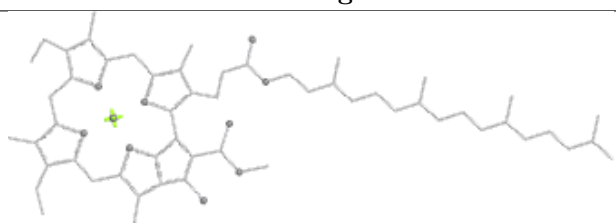
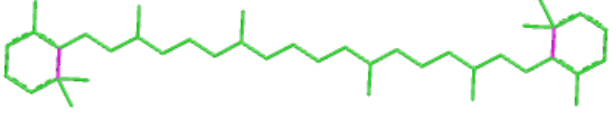
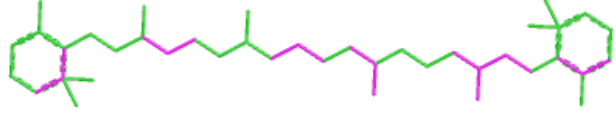
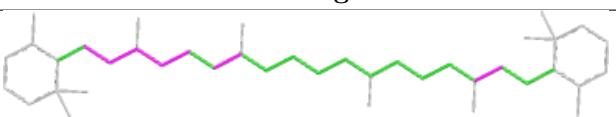
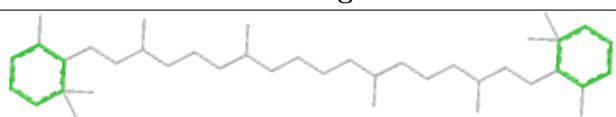
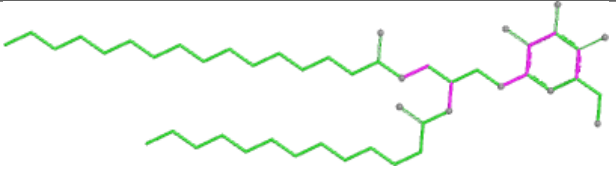
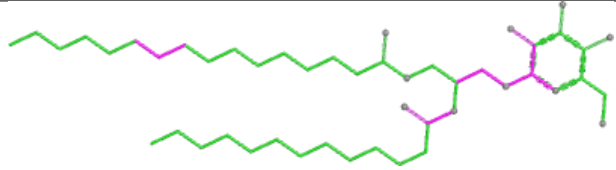
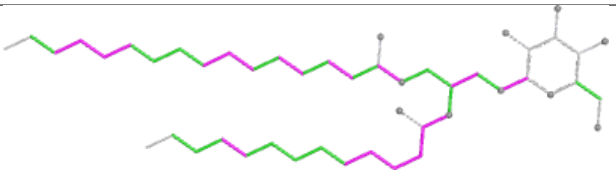
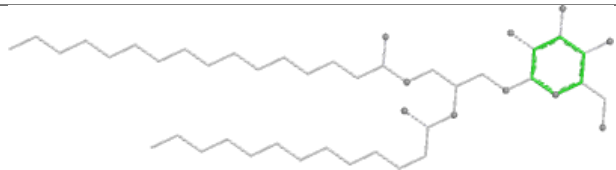


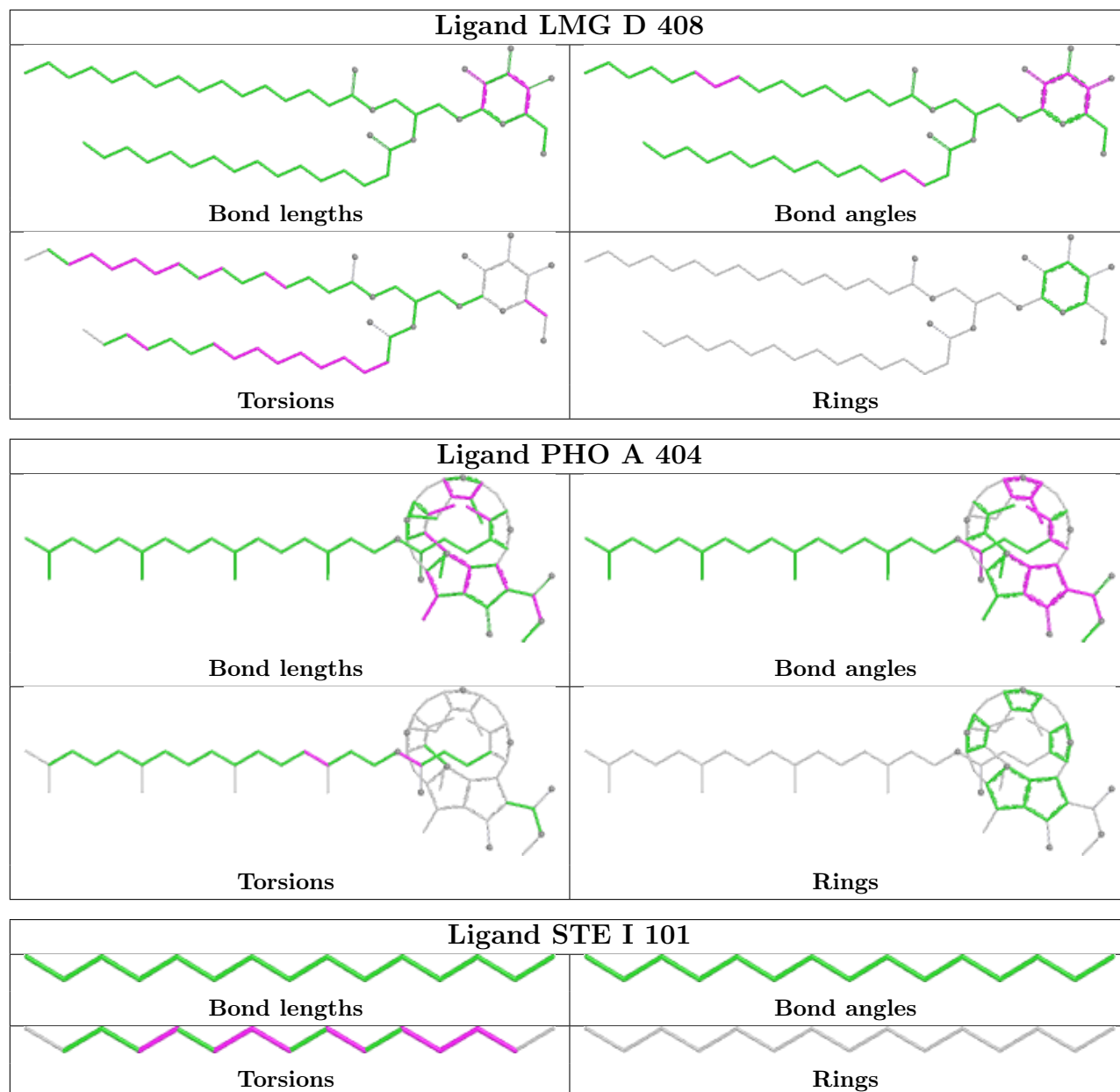
Ligand CLA B 602**Ligand BCR Z 101****Ligand CLA c 509**

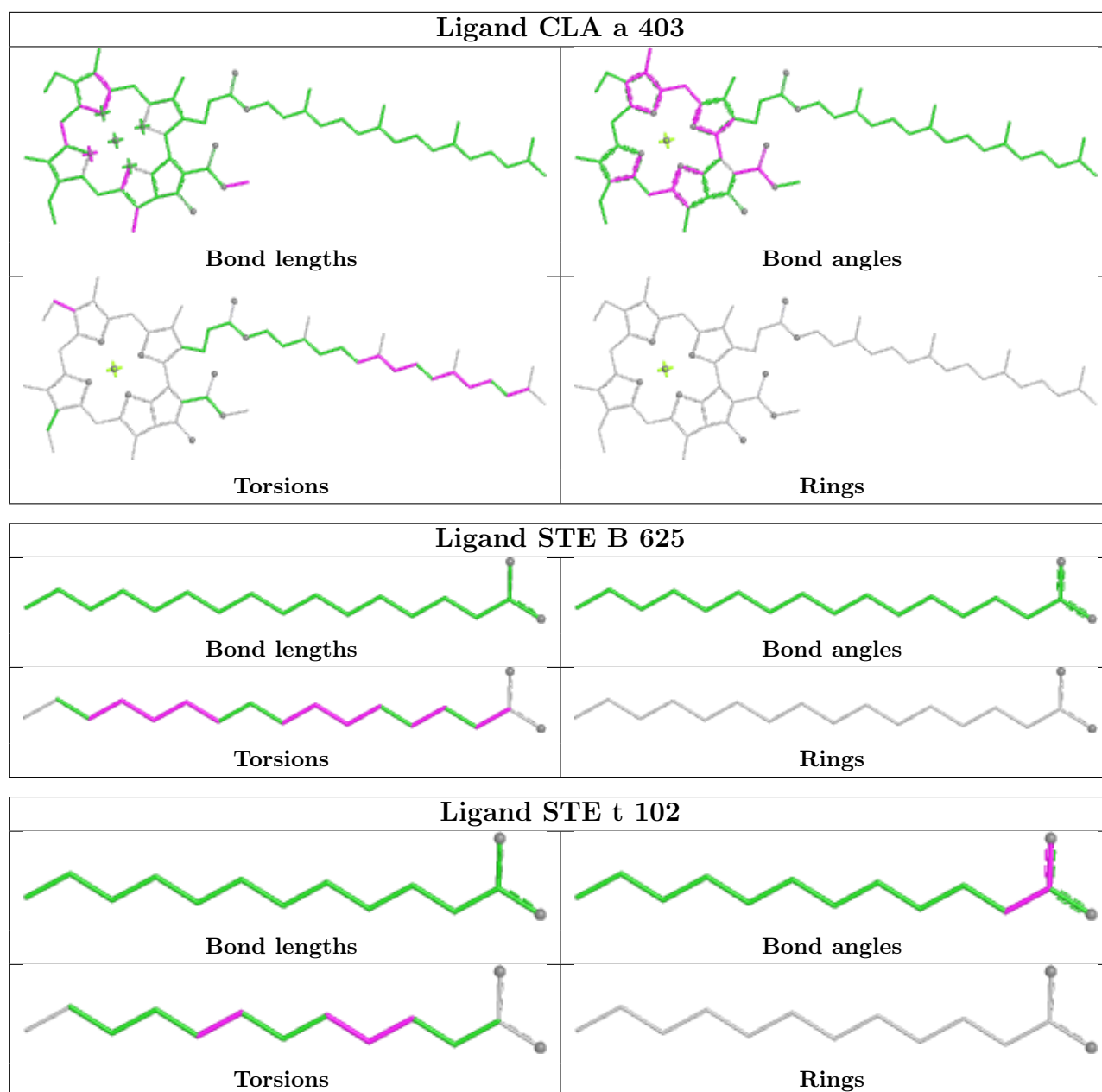


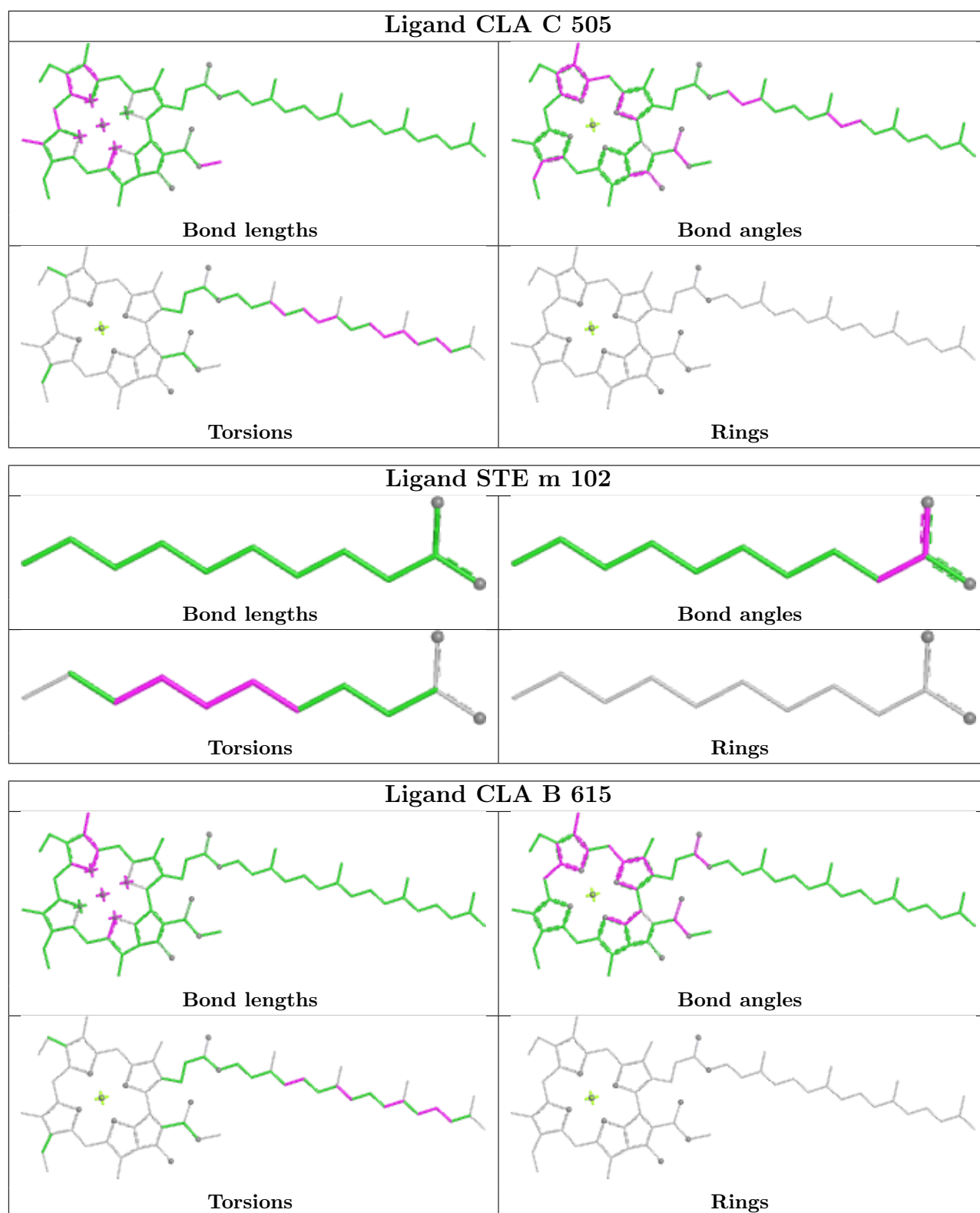


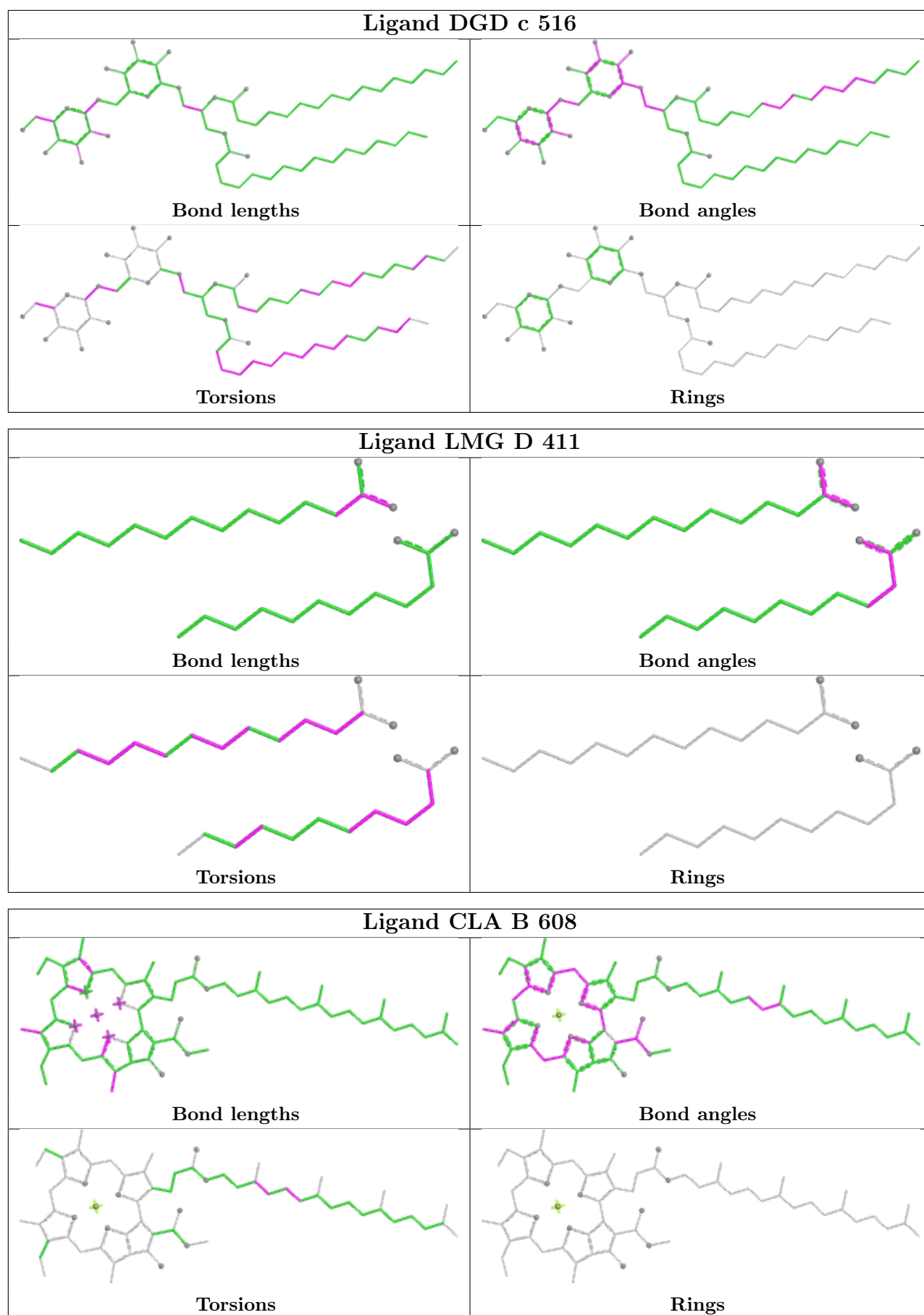


Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

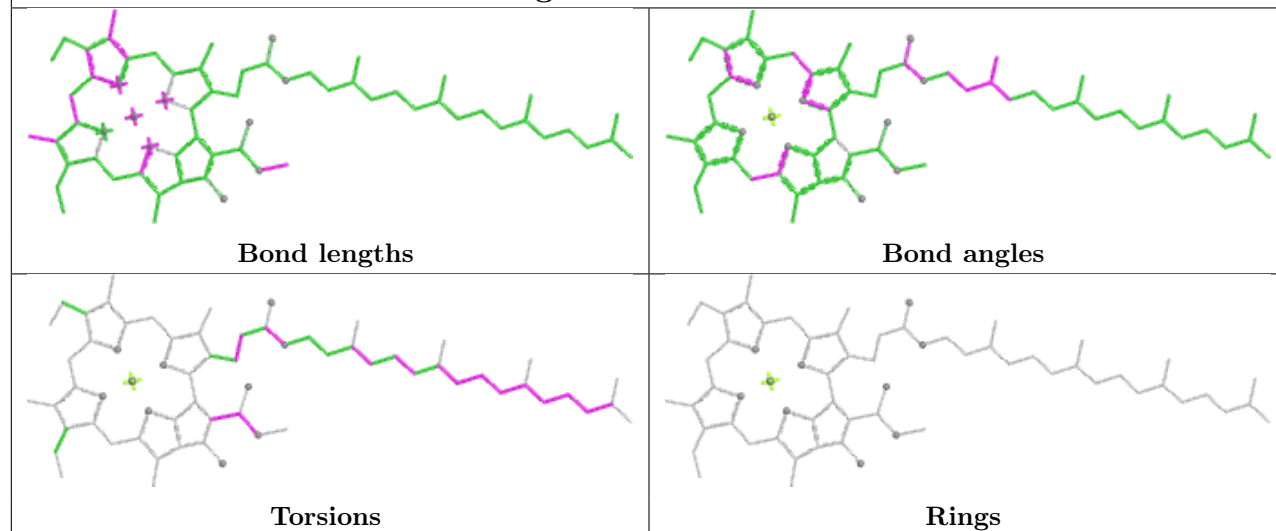




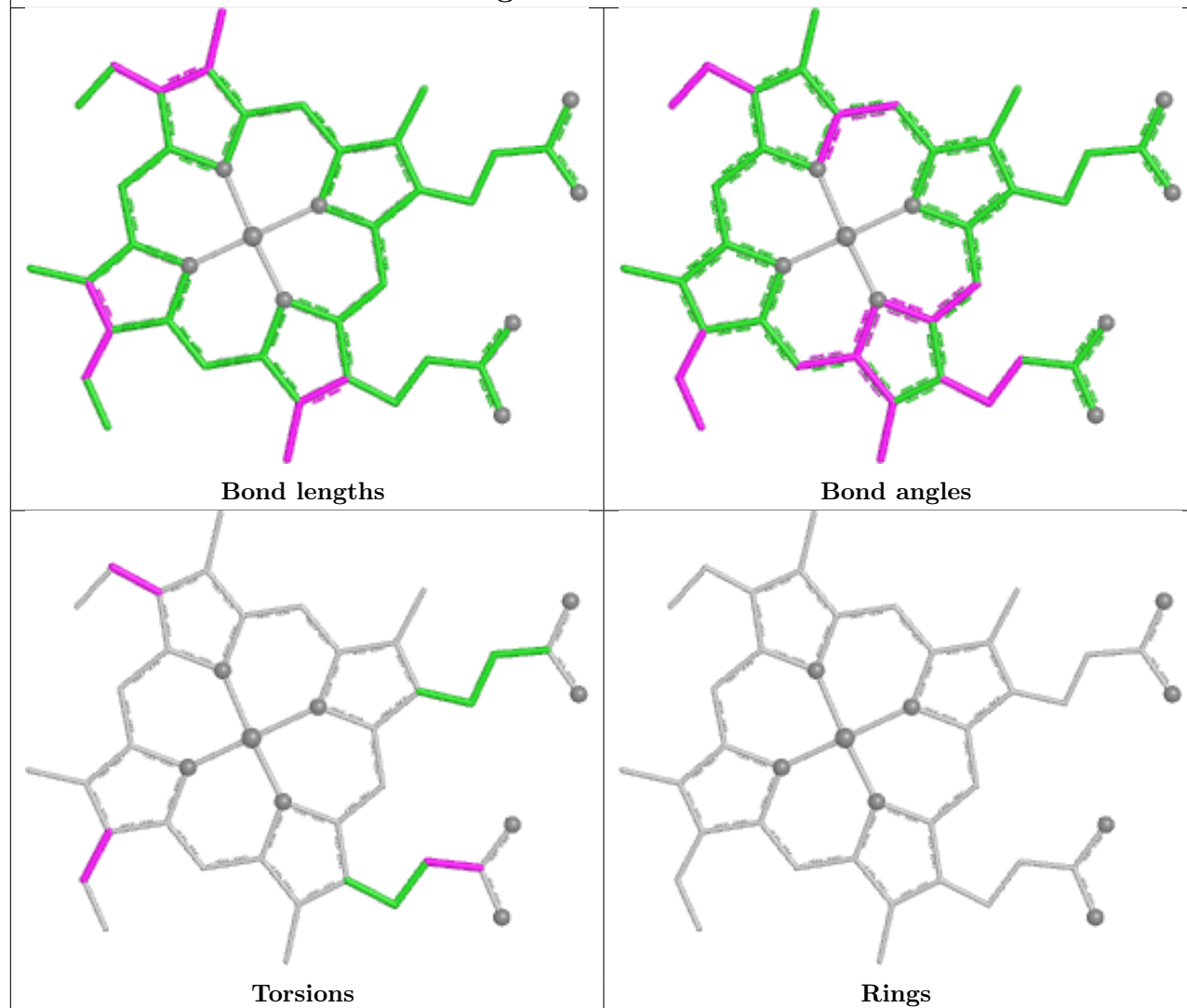




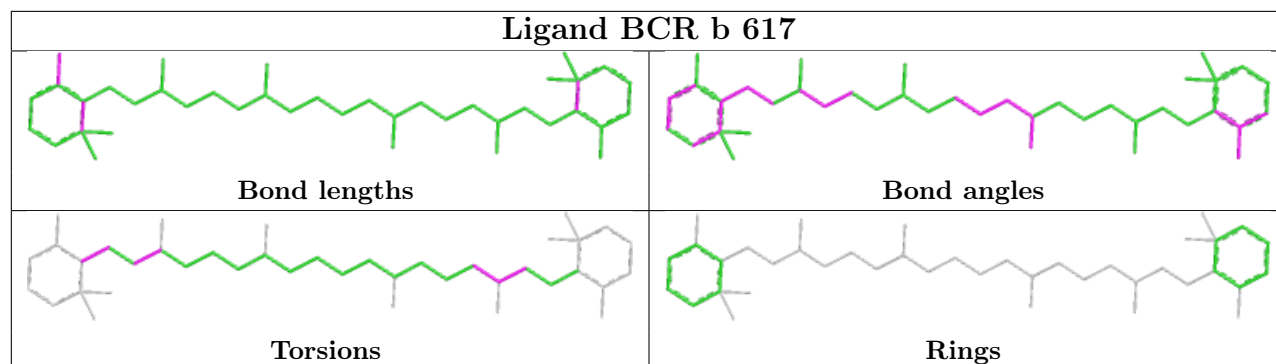
Ligand CLA b 614



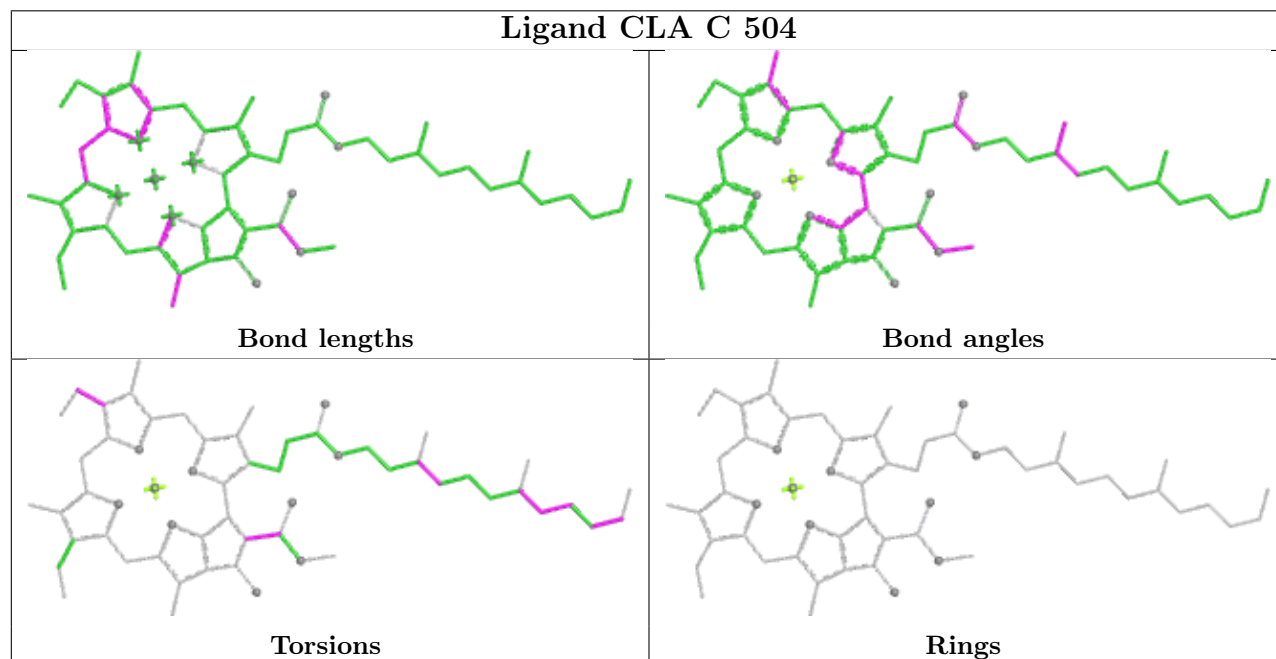
Ligand HEC v 201



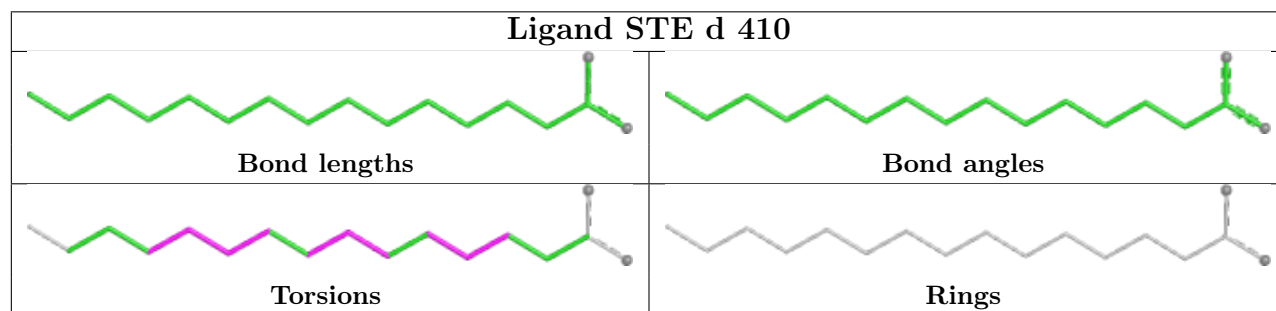
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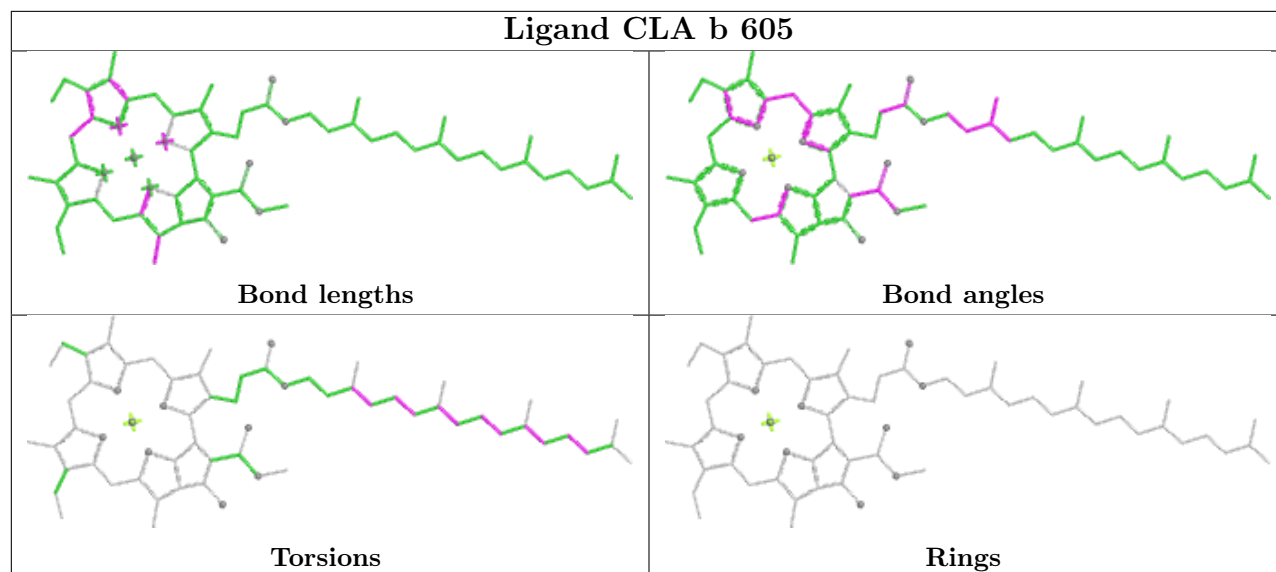
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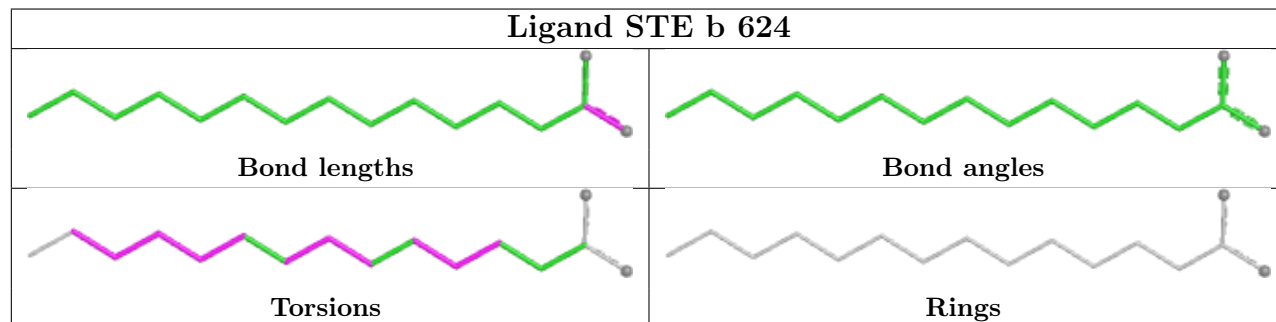
Ligand STE d 410



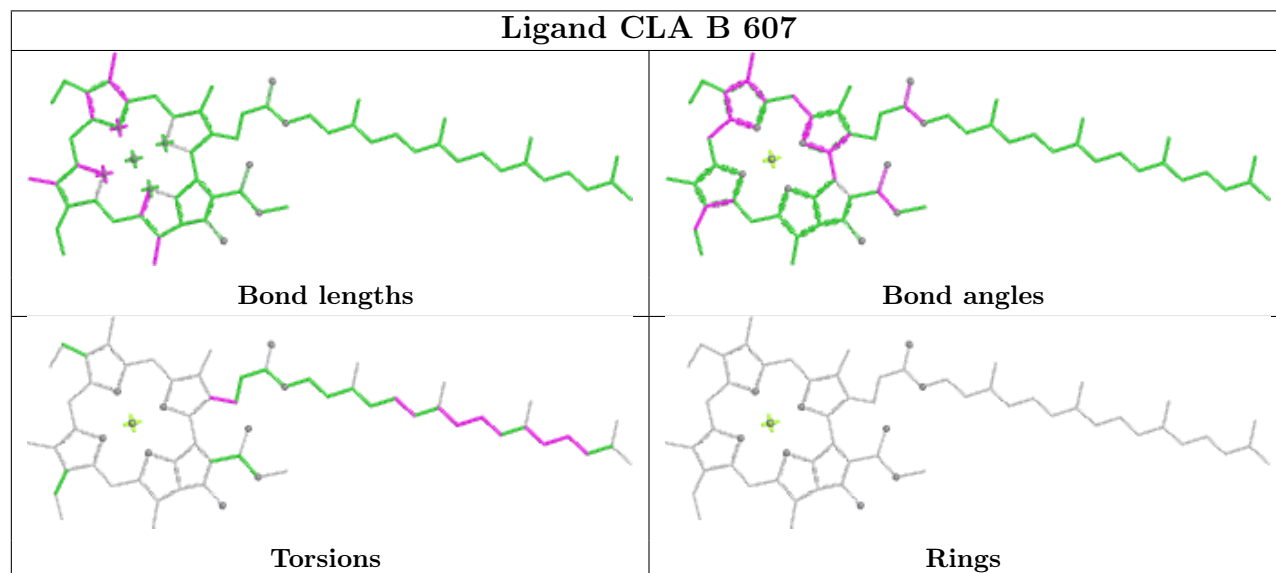
Ligand CLA b 605



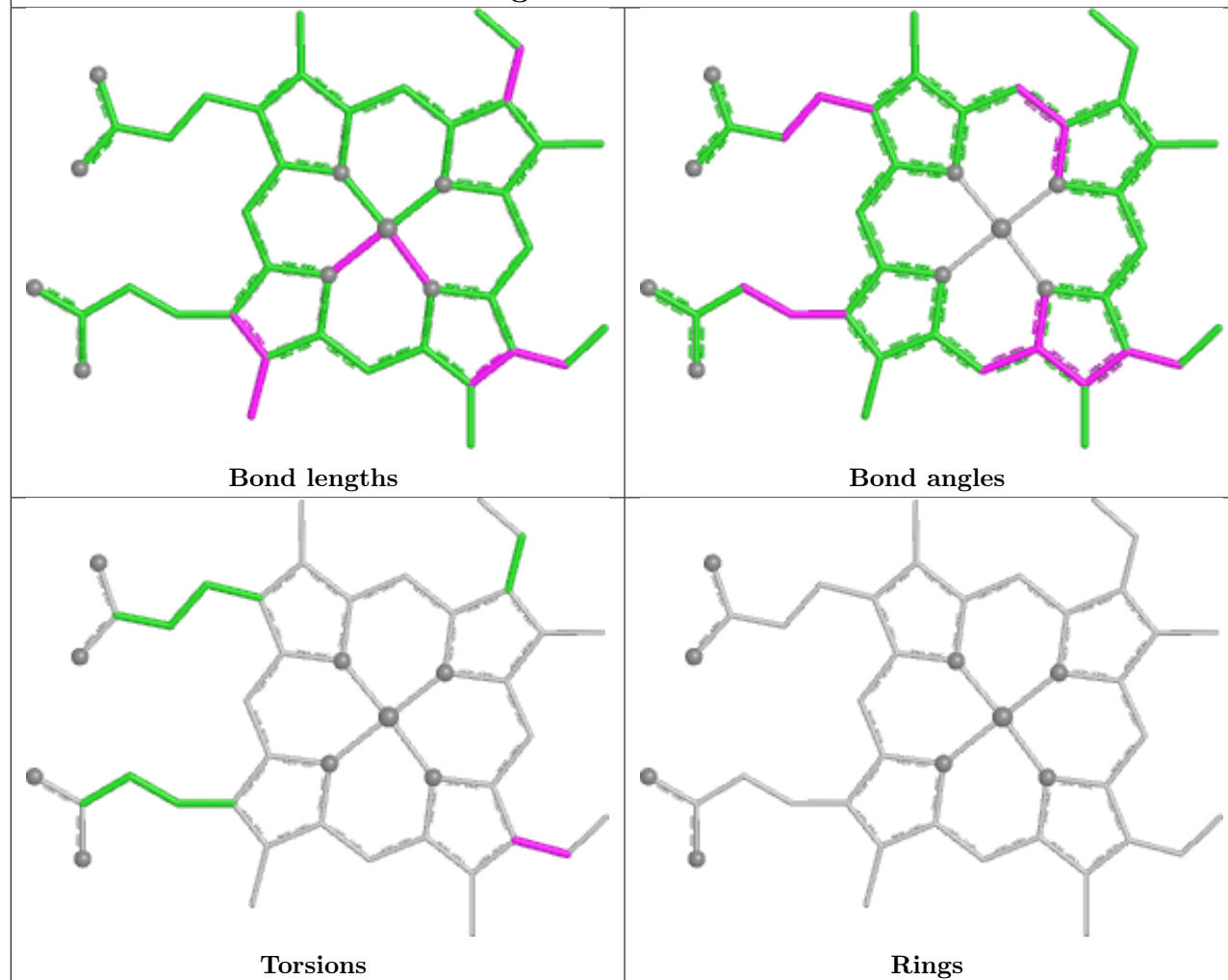
Ligand STE b 624



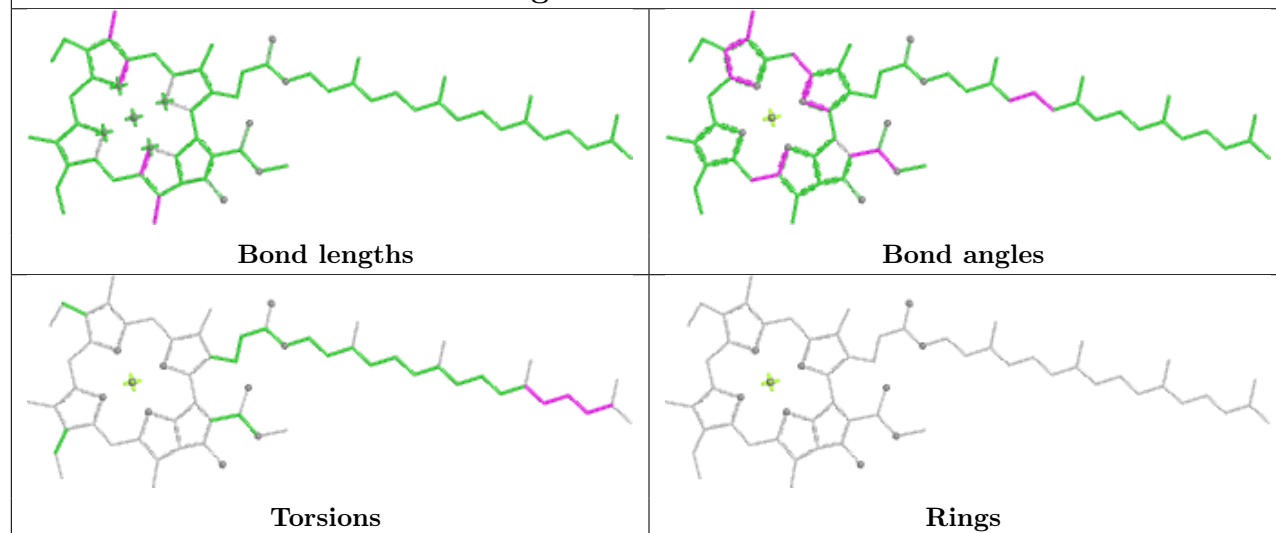
Ligand CLA B 607

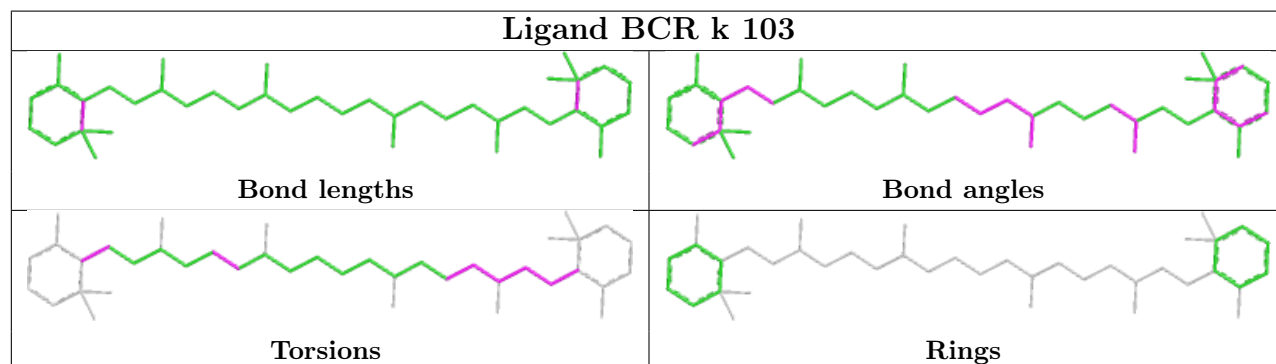
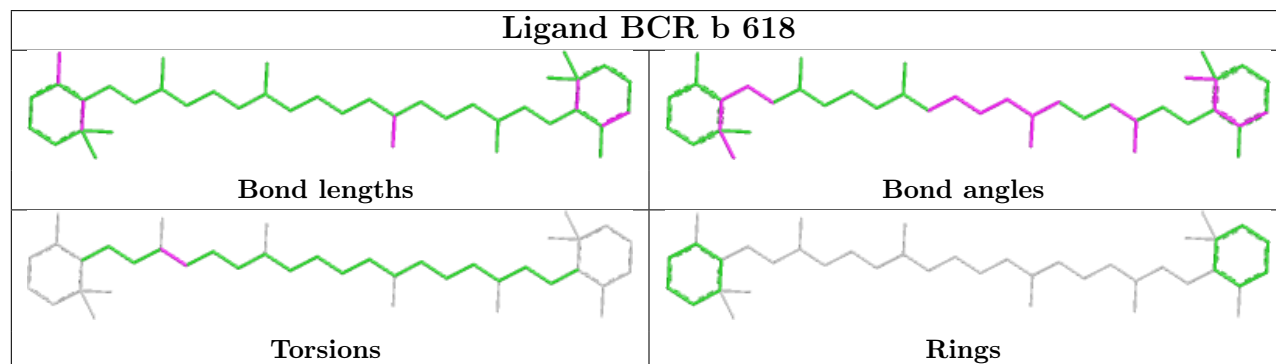
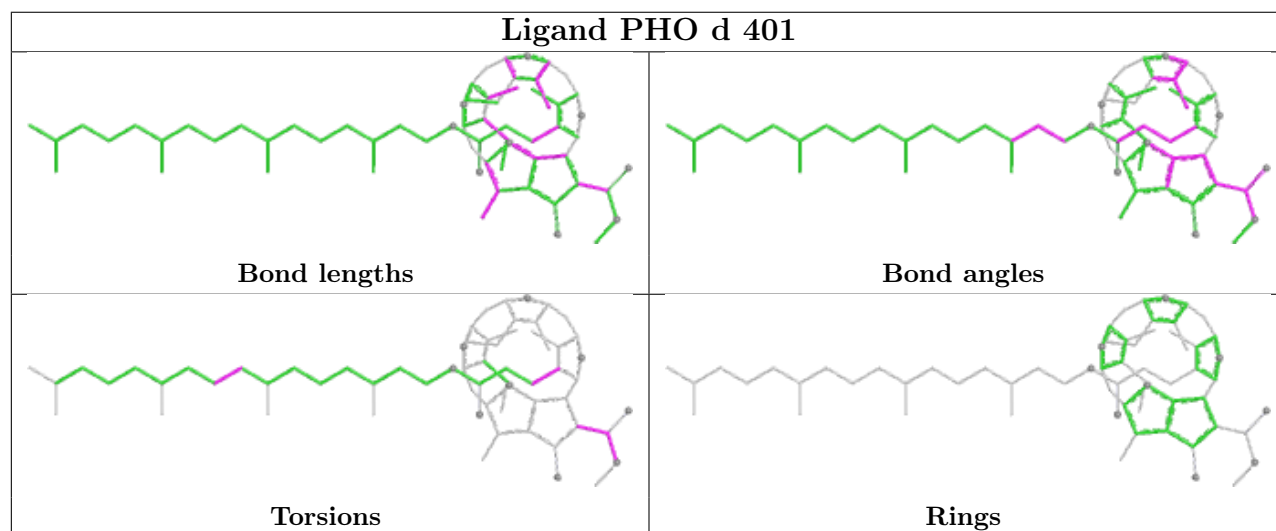
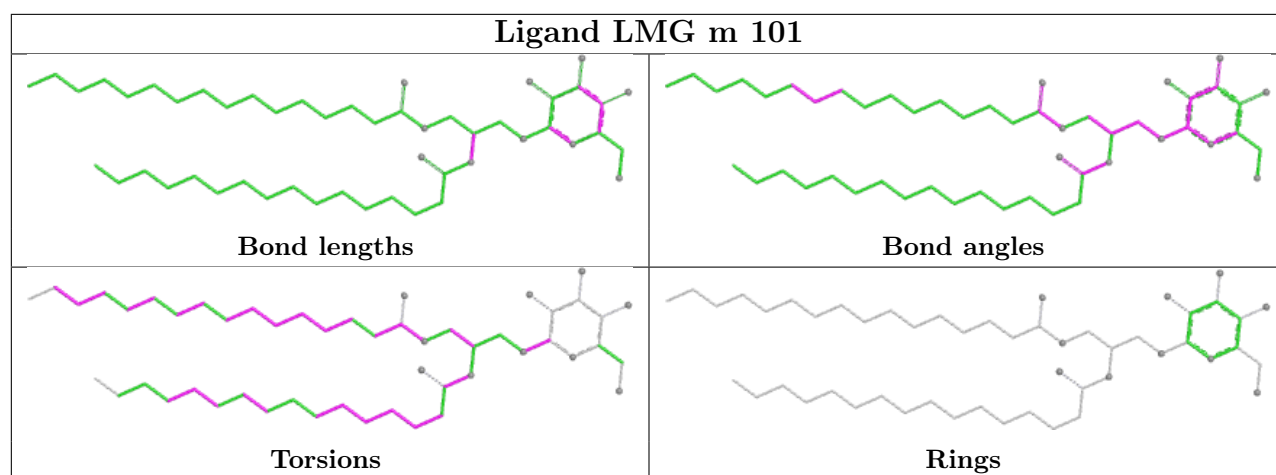


Ligand HEM e 101

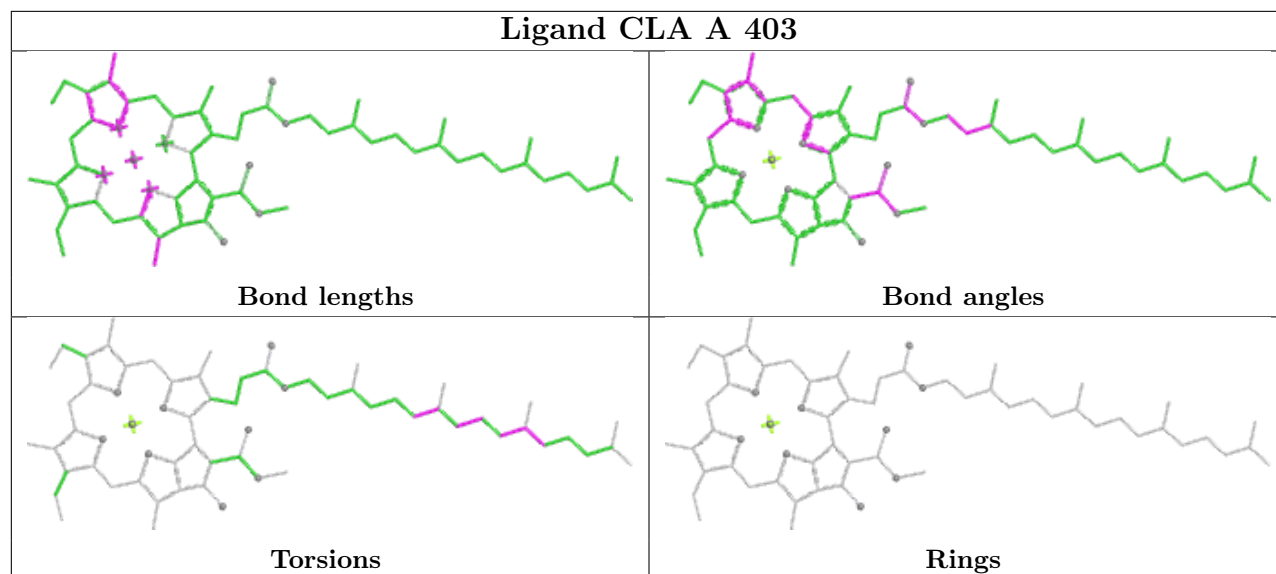


Ligand CLA D 404

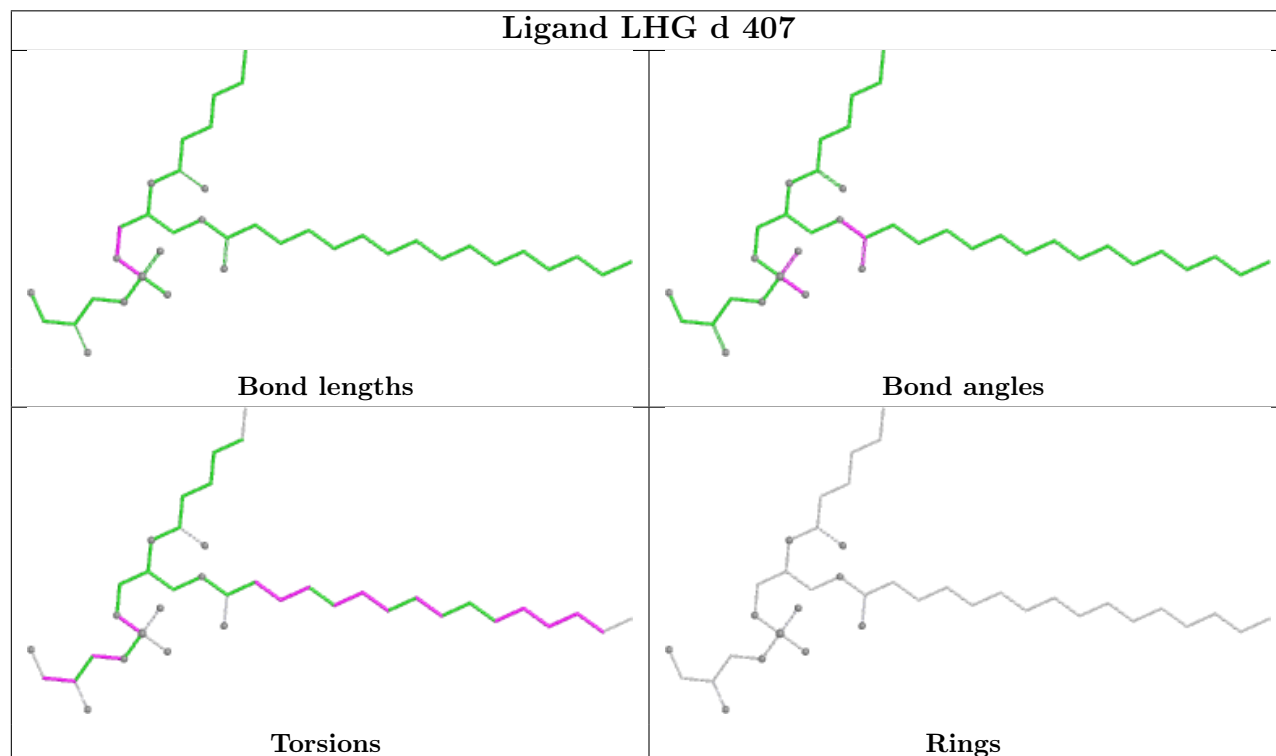


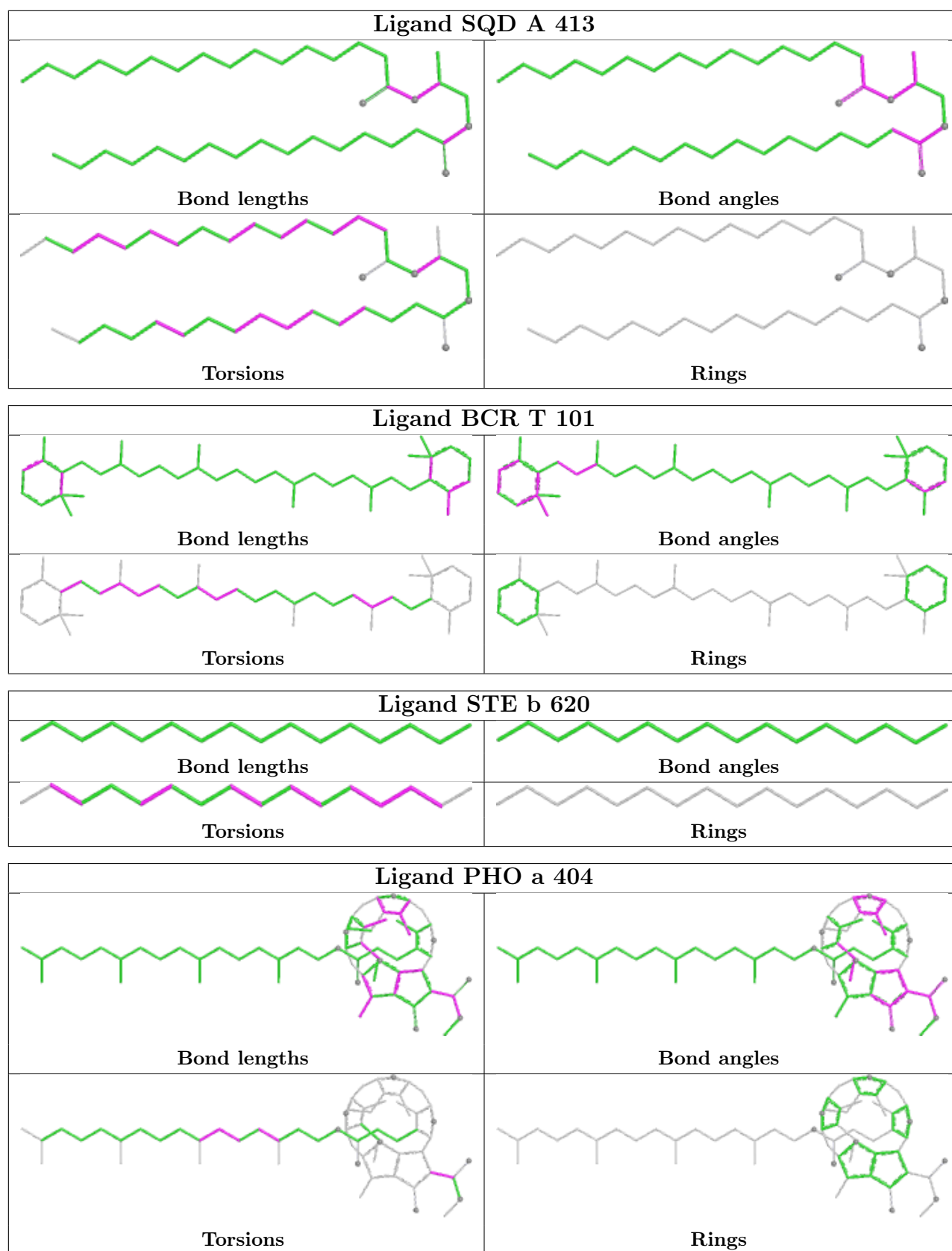


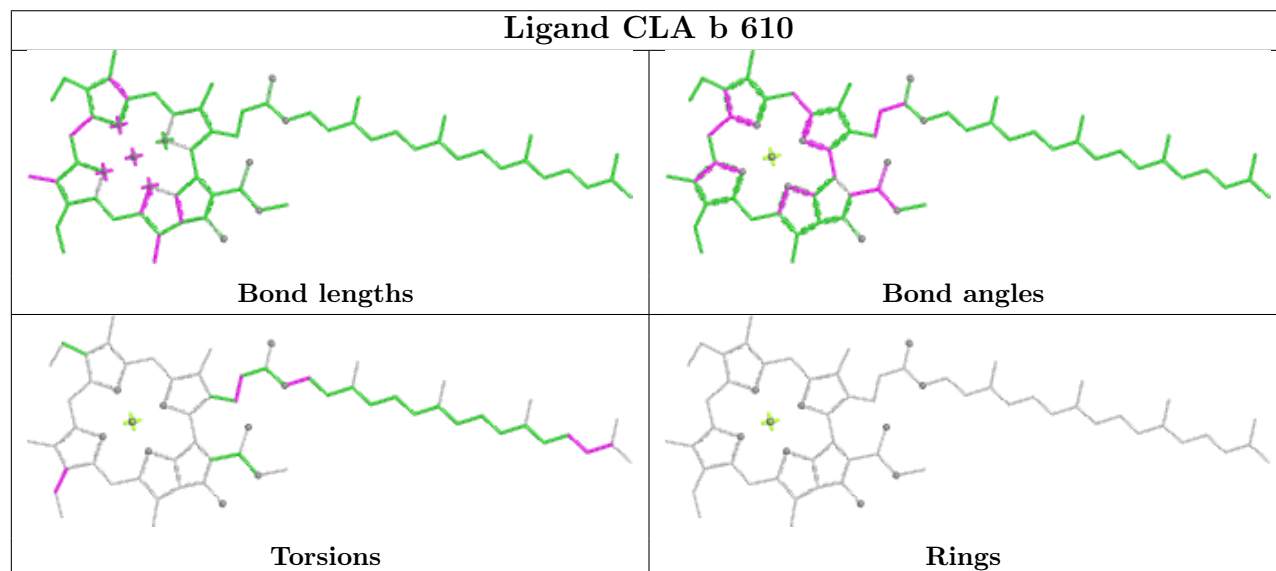
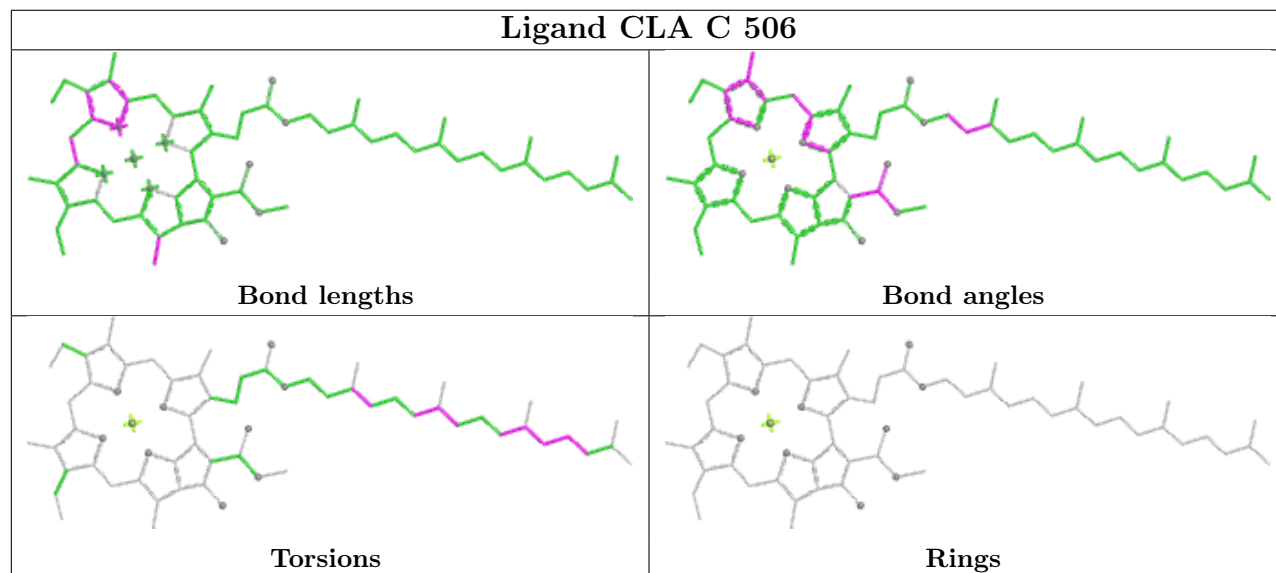
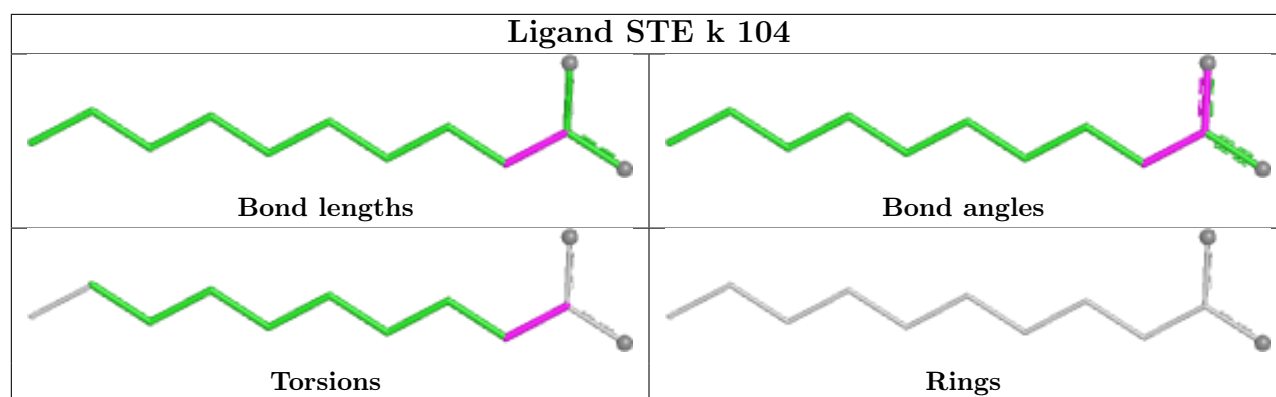
Ligand CLA A 403

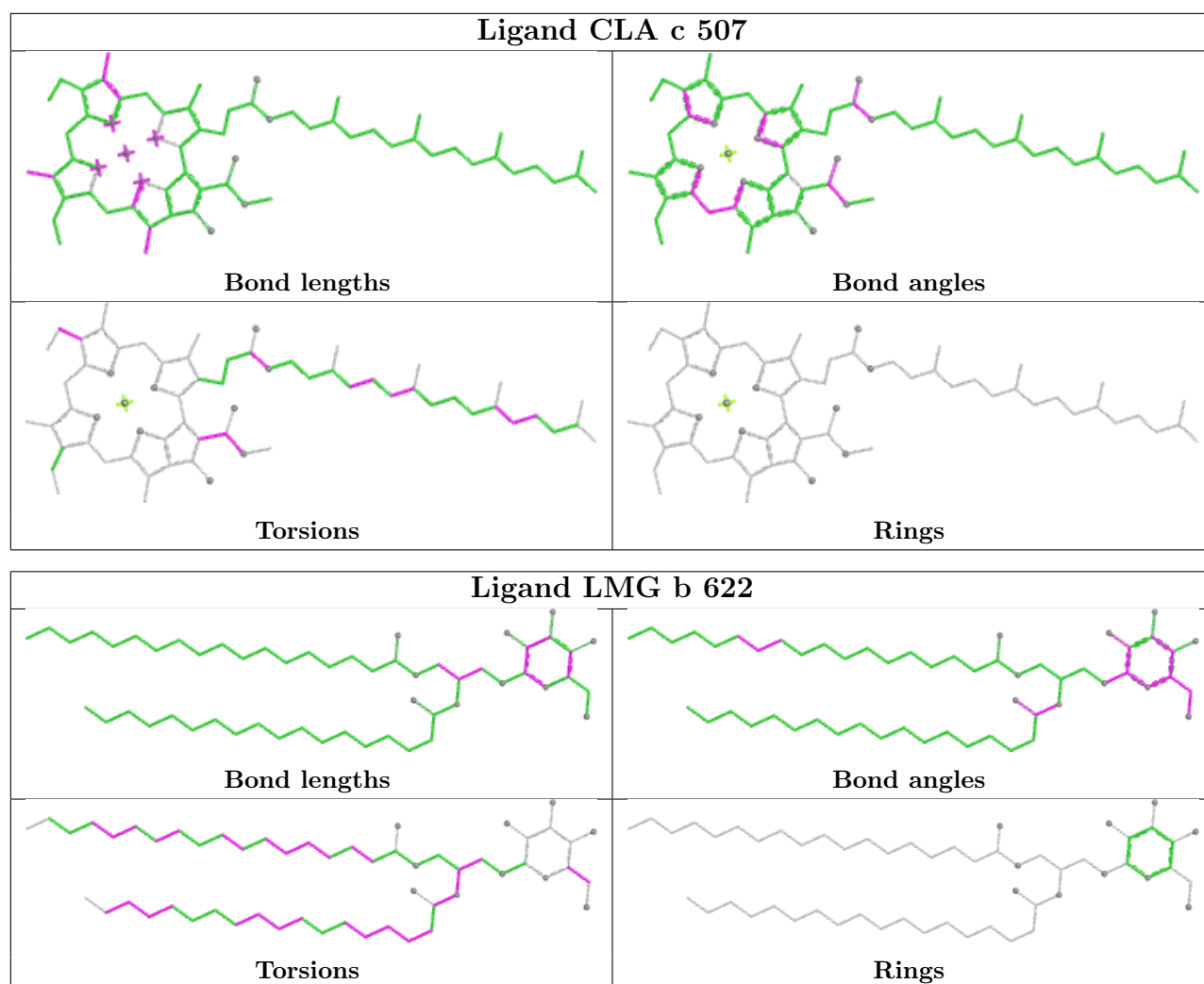


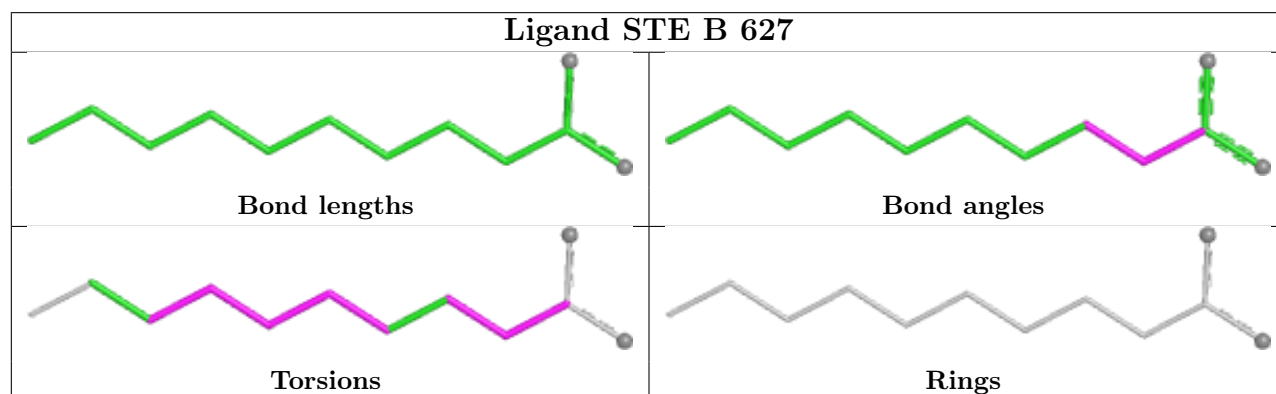
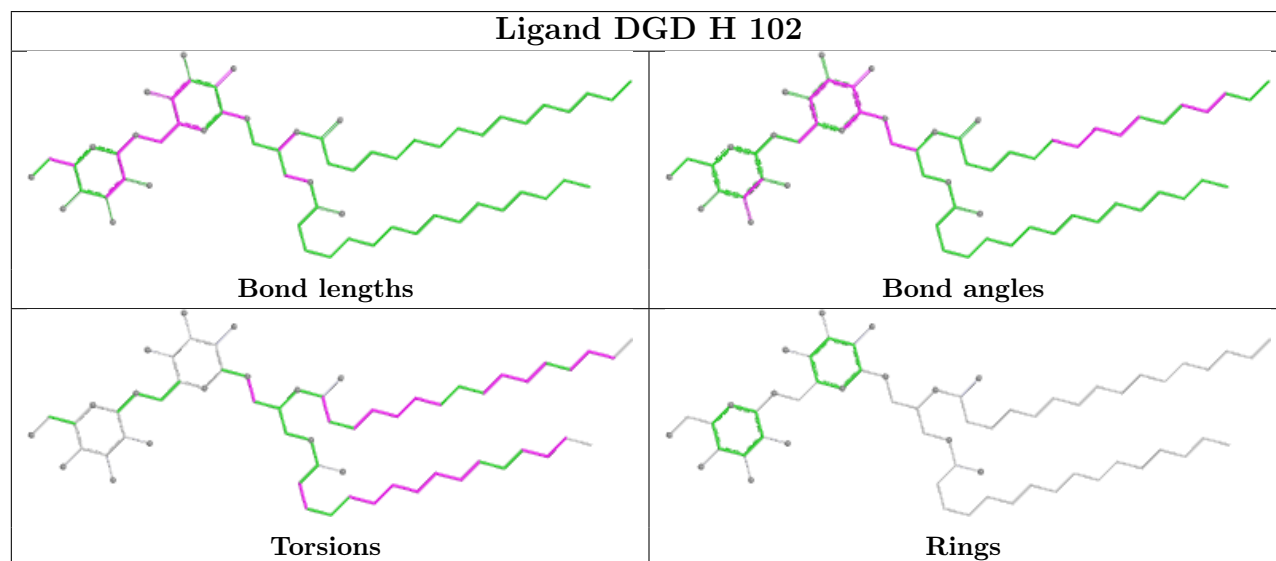
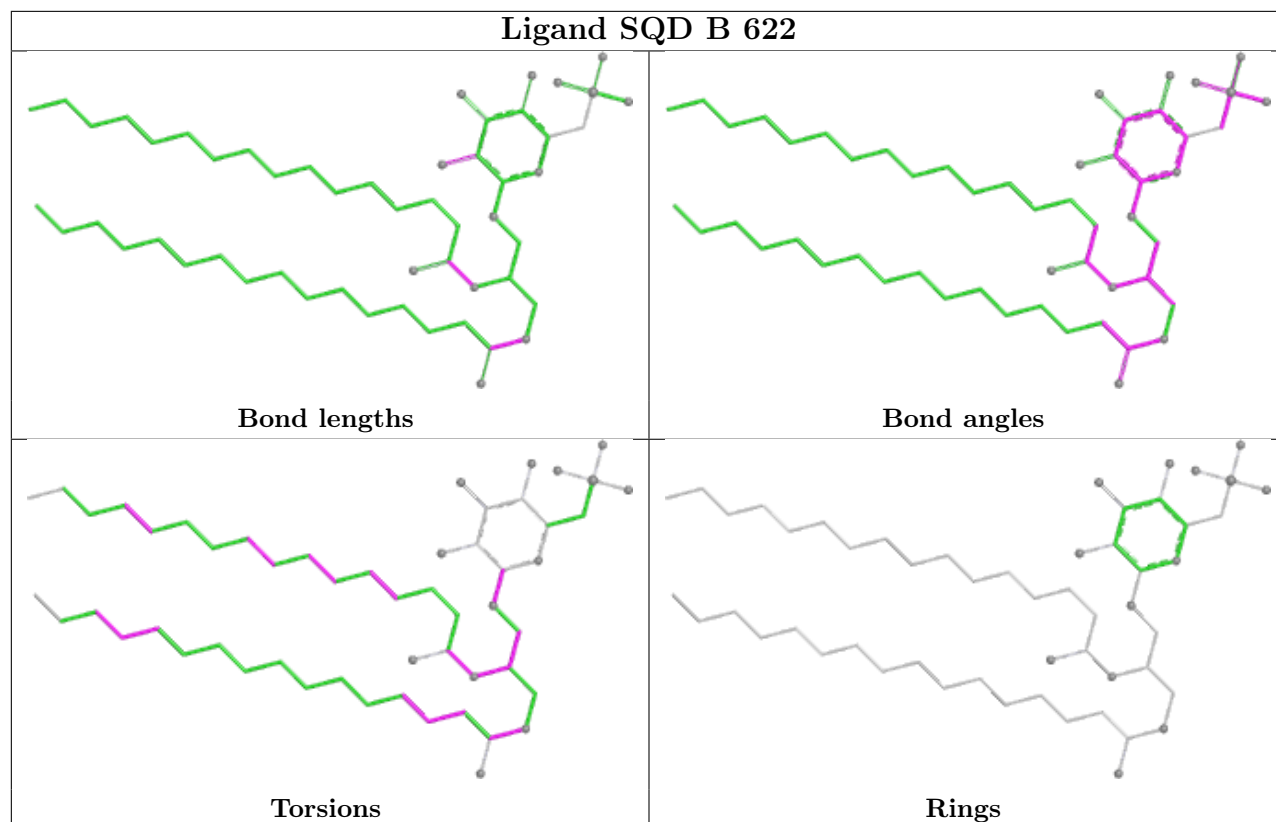
Ligand LHG d 407



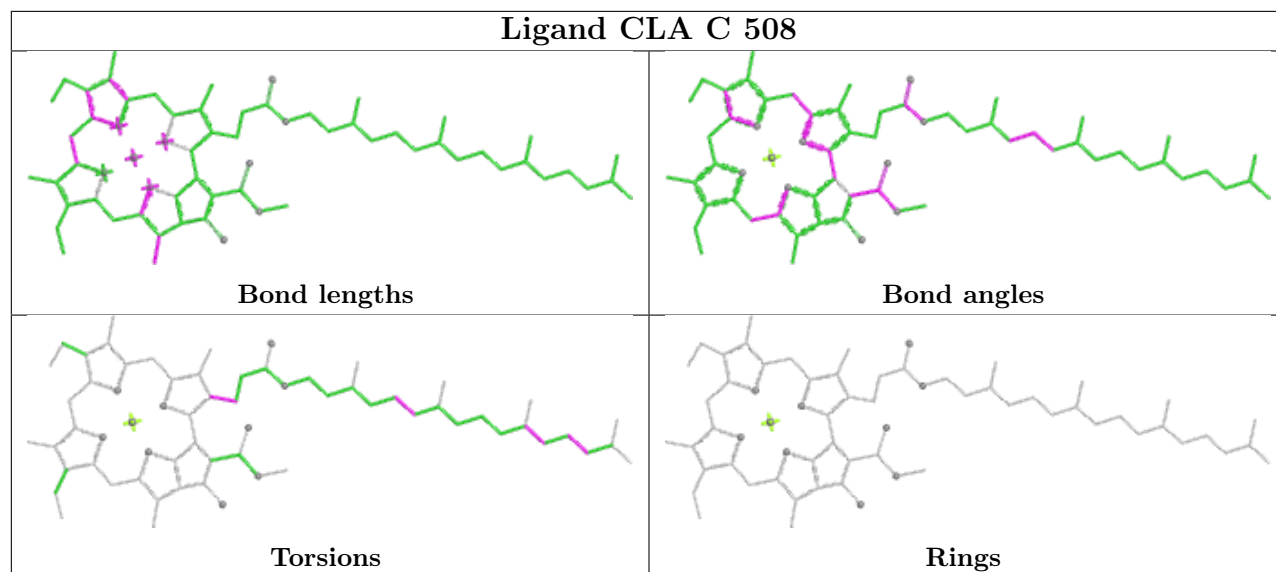




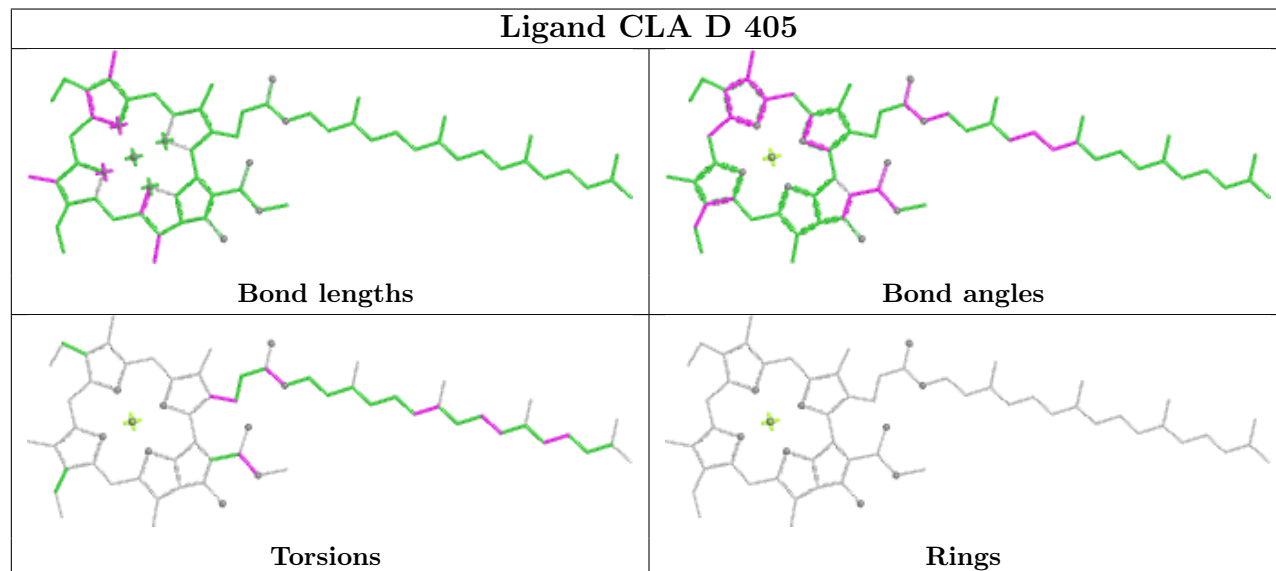




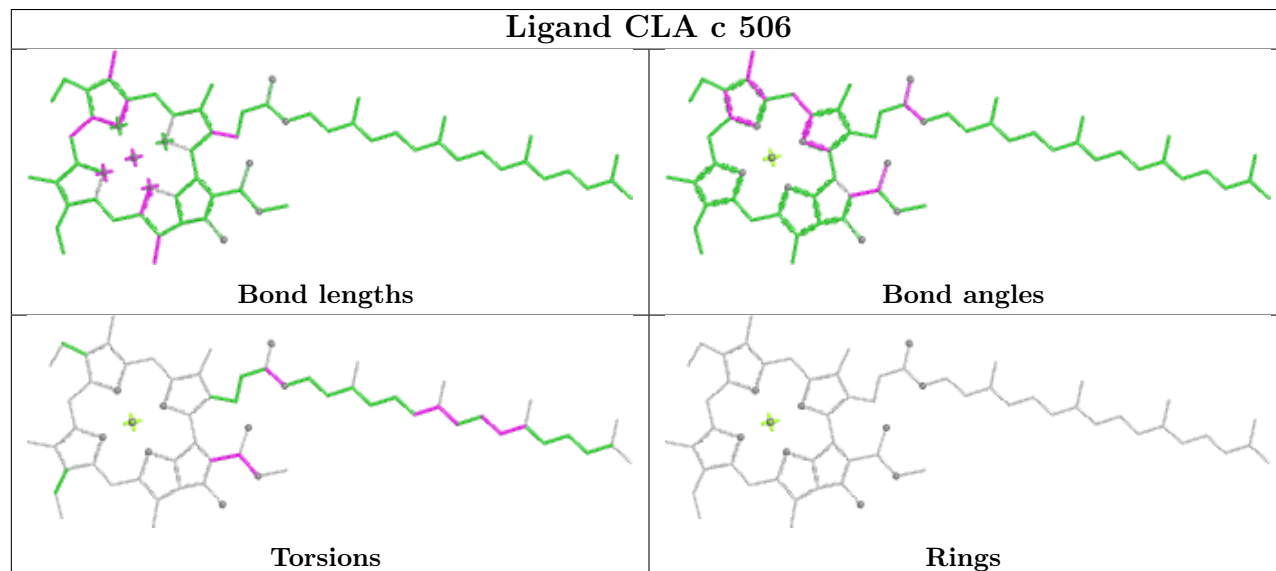
Ligand CLA C 508

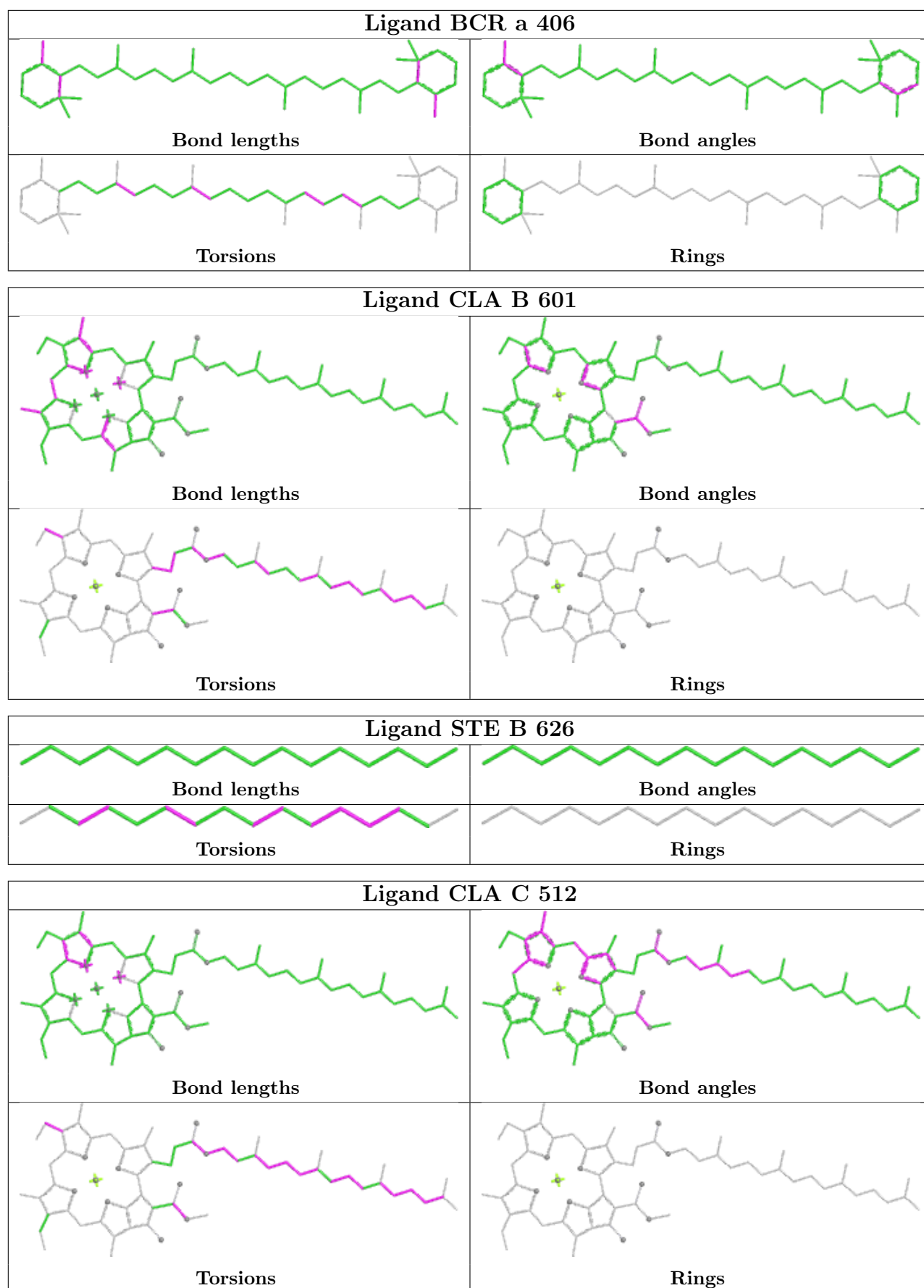


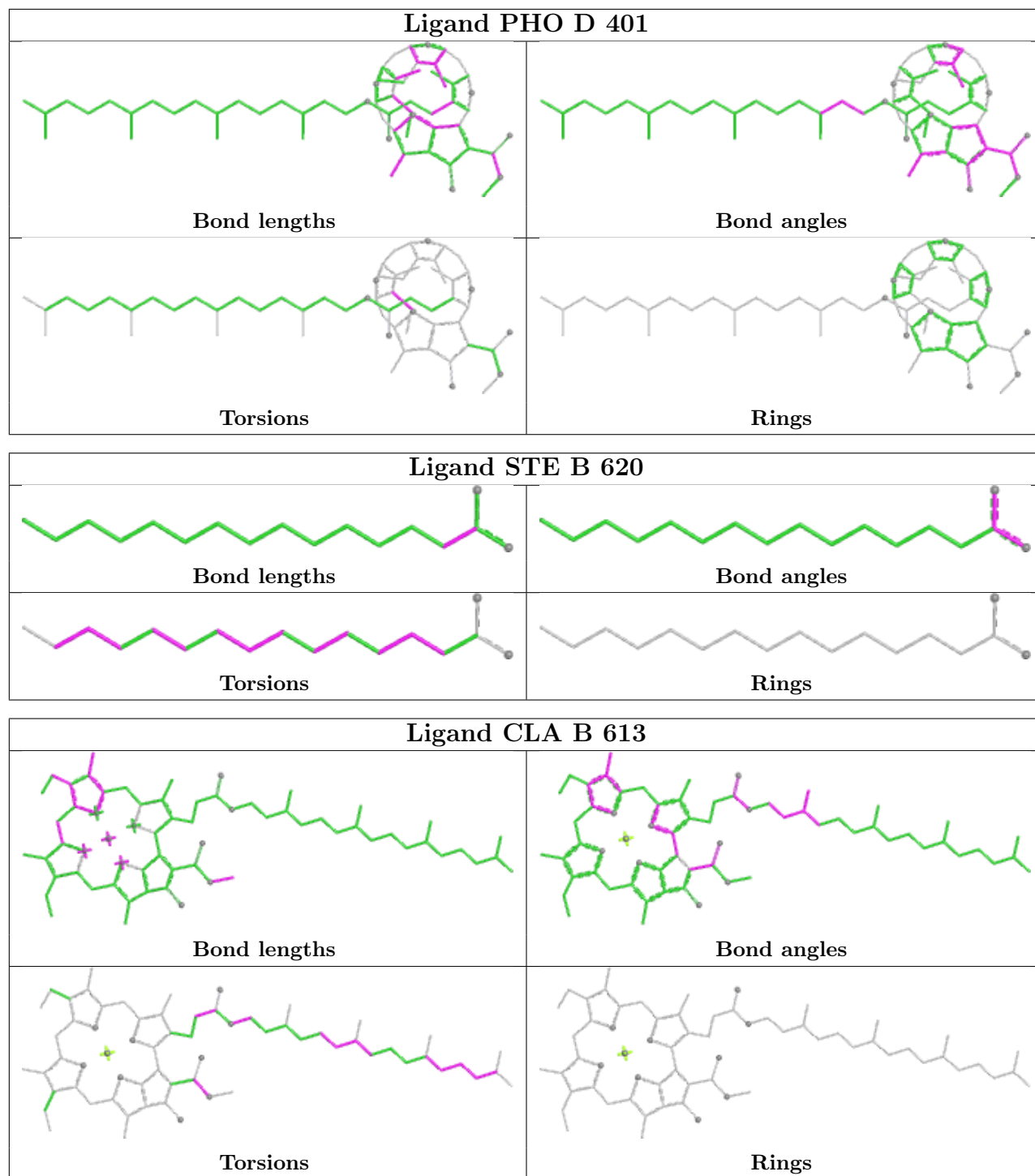
Ligand CLA D 405

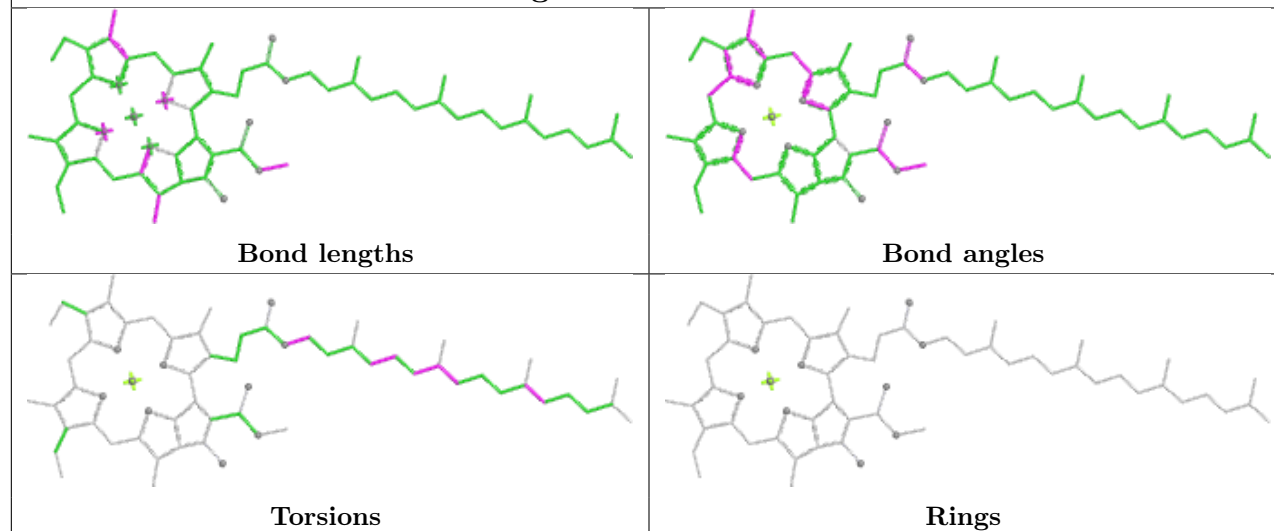
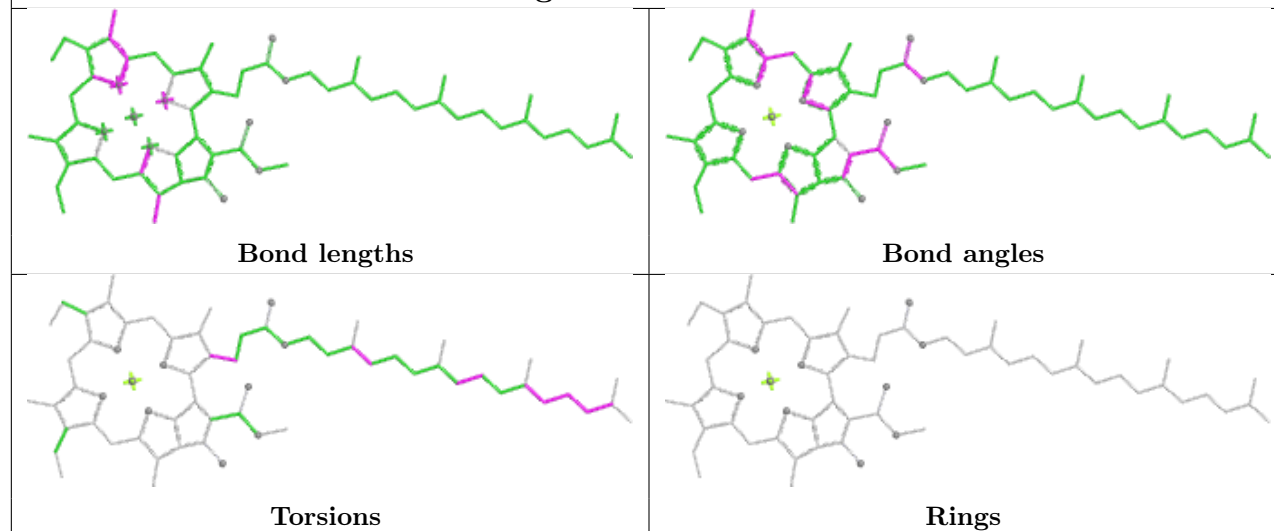


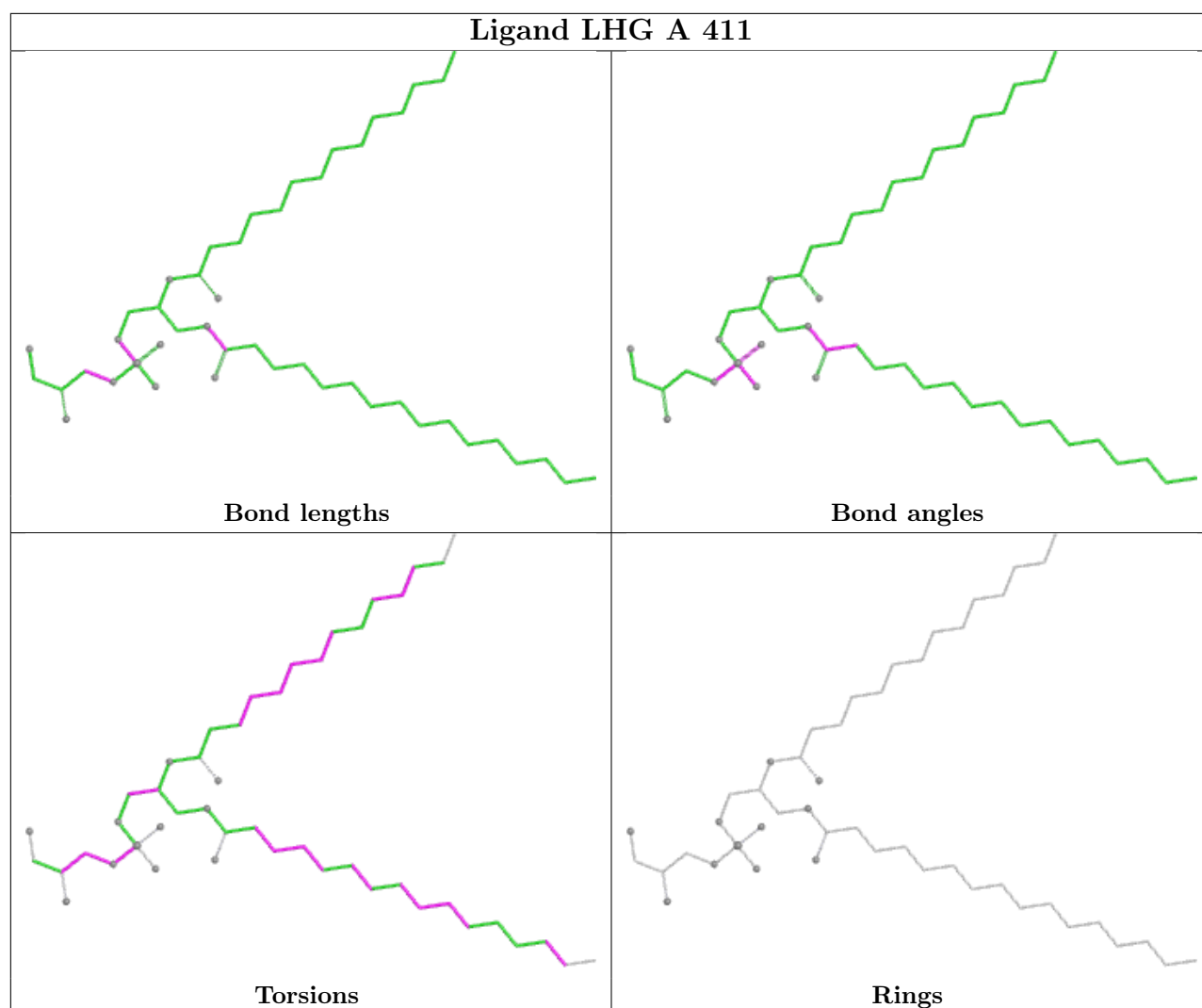
Ligand CLA c 506

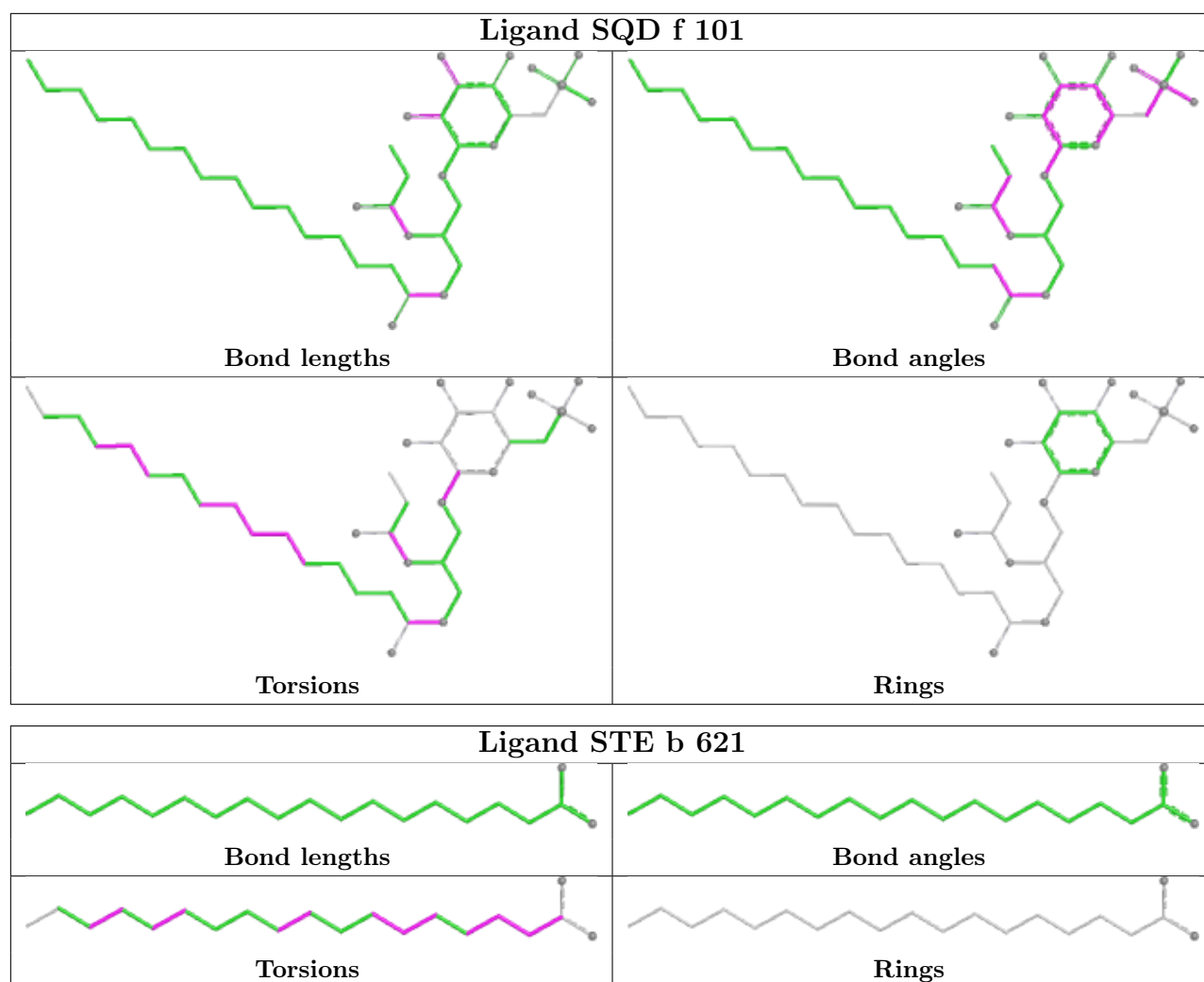






Ligand CLA D 403**Ligand CLA b 611**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.